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Doctoral Thesis

Optimisation Methodologies for the Design and Planning of Water Systems

Author:
Mariya Koleva

Supervisors:
Prof. Lazaros Papageorgiou
Dr. Craig Styan

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Declaration of Authorship

I, Mariya Koleva, declare that this thesis titled, 'Optimisation Methodologies for the Design and Planning of Water Systems' and the work presented in it are my own. I confirm that:

- This work was done wholly or mainly while in candidature for a research degree at this University.
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- Where I have consulted the published work of others, this is always clearly attributed.
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"Art and science have their meeting point in method."

Earl Edward George Bulwer-Lytton

UNIVERSITY COLLEGE LONDON

Abstract

Faculty of Engineering Sciences
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Doctor of Philosophy

Optimisation Methodologies for the Design and Planning of Water Systems

by Mariya Koleva

This thesis addresses current topics of design and planning of water systems from water treatment units to a country-wide resources management schemes. The methodologies proposed are presented as models and solution approaches using mathematical programming, and mixed integer linear (MILP) and non-linear (MINLP) programming techniques.

In Part I of the thesis, a synthesis problem for water treatment processes using superstructure optimisation is studied. An MINLP model is developed for the minimisation of water production cost considering physicochemical properties of water and operating conditions of candidate technologies. Next, new alternative path options are introduced to the superstructure. The resulting MINLP model is then partially linearised (plMINLP) and also presented as a mixed integer linear fractional programming (MILFP) model in order to improve the convergence of the optimisation model. Various linearisation and approximation techniques are developed. As a solution procedure to the fractional model, a variation of the Dinkelbach's algorithm is proposed. The models are tested on theoretical examples with industrial data.

In Part II, an optimisation approach formulated as a spatially-explicit multi-period MILP model is proposed for the design of planning of water resources at regional and national scales. The optimisation framework encompasses decisions such as installation of new purification plants, capacity expansion, trading schemes among regions and pricing, and water availability under climate change. The objective is to meet water demand while minimising the total cost associated with developing and operating the water supply chain. Additionally, a fair trade-off between the total cost and reliability of the supply chain is incorporated in the model. The solution method is applied based on game theory using the concept of Nash equilibrium. The methodology is implemented on a case study based on Australian water management systems.

Impact Statement

Water is used not only for drinking but it is also virtually embedded in food, energy and clothes. It is predicted that water demand will increase by 55% by 2050. Thus, the well-known supply = demand rule has begun to dis-balance in favour of demand. As a consequence, future water shortages can drive to global political and human life crises.

One direction of mitigating those catastrophes is reflected in the acknowledged need for efficient and cost cutting methods to assist in holistic decision making of water management. Solely the capital investment on water infrastructure a year is estimated at 41 bnUSD in USA and 5 bnGBP in the UK and yet to rise.

In 2013 the aforementioned necessity gave birth to the project which aimed to develop methodologies for water management, implemented using mathematical programming and optimisation theory. Both of the approaches rest on interdisciplinary research which combines technical, economic, environmental and regulatory aspects as to allow more comprehensive representation of practices in reality. The two axes of the project address two different scales of water management: treatment processes and supply chain.

In the first approach, the best technology path is selected for pre-specified initial water conditions and final use product which must be in compliance with standards set by regulatory authorities. The driving force behind the selection is the running and capital cost of the system design. Alongside with purification units, their operating conditions for the most efficient usage of the flowsheet are also output. Such a tool will be able to deliver preliminary design results within 5-6 minutes, which is particularly useful for water engineers and consultants, who are involved in months-long process of initial screening of best available technologies.

The second approach is developed to assist governments and authorities to make more informed water infrastructure decisions in a financially viable manner. The framework takes into account climatic changes, such as el Niño oscillations, supply reliability, trading and governmental targets. A tool of this kind has the power to justify capacity installations and expansions decisions, location and type of purification plant necessary, amounts and directions of trading, and how reliable the designed system would be by seeking for the minimum incurring investment and maintenance costs. The framework provides a systematic long-term planning which again provides solution in minutes.

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Abbreviations

CLR	**CL**a**R**ification technologies
MSF	**M**ulti-**S**tage **F**lash
MEF	**M**ulti-**E**ffect **D**istillation
VP	**V**apour **C**ompression
MF	**M**icrofiltration
UF	**U**ltrafiltration
NF	**N**nanofiltration
RO	**R**everse **O**smosis
ED	**E**lectrodialysis
DAF	**D**issolved **A**ir **F**loatation
SED	**S**edimentation
LP	**L**inear **P**rogramming
NLP	**N**on-**L**inear **P**rogramming
MINLP	**M**ixed **I**nteger **N**on-**L**inear **P**rogramming
plMINLP	**p**artially **l**inearised **M**ixed **I**nteger **N**on-**L**inear **P**rogramming
MILP	**M**ixed **I**nteger **L**inear **P**rogramming
MILFP	**M**ixed **I**nteger **L**inear **F**ractional **P**rogramming
SA	**S**outh **A**ustralia
VIC	**VIC**toria
NSW	**N**ew **S**outh **W**ales
QLD	**Q**ueens**L**an**D**
WA	**W**estern **A**ustralia
NT	**N**orthern **T**erritory
TAS	**TAS**mania
ACT	**A**ustralian **C**apital **T**erritory

GAMS	**G**eneral **A**lgebraic **M**odelling **S**ystem
TDS	**T**otal **D**issolved **S**olids
TSS	**T**otal **S**uspended **S**olids
COD	**C**hemical **O**xygen **D**demand
B	**B**oron
MMF	**M**ulti-**M**edia **F**iltration
MIP	**M**ixed **I**nteger **P**rogramming
SC	**S**upply **C**hain(s)
DOC	**D**issolved **O**rganic **C**arbon
WNS	**W**ater **N**etword **s**ystem
ANOVA	**A**nalysis **o**f **V**ariance

Nomenclature

Indices

c	contaminants
g, g'	states with a maximum number of states G^{max}
i, i'	resources (sw, gw, dw, uw), see Chapter 4 and Chapter 5
i, j	passes, see Chapter 2
j	discretisation points
k	discrete options for separable approach
l	capacity option levels for installation or expansion, see Chapter 4 and Chapter 5
l	positions in multiparametric disaggregation
m	positions in piecewise approximation with a final position M^{max}, see Chapter 3
m	trading prices options, see Chapter 4 and Chapter 5
p	plants
q	parallel technologies for CLR, see Chapter 2 and Chapter 3
q	seasonal time periods with a maximum number of seasons Q^{max}, see Chapter 4 and Chapter 5
r	positions in piecewise reformulation
s	parallel technologies for CLR, see Chapter 2
s	stages, see Chapter 3

t technologies, see Chapter 2 and Chapter 3

t yearly time periods with a maximum number of years T^{max}, see Chapter 4 and Chapter 5

z positions in multiparametric disaggregation

Sets

$\bar{I}_q$ a set of passes and stages of parallel technologies, q, for CLR

$\bar{I}_s$ a set of passes of parallel technologies, s, for CLR

$\eta_{igg'}$ a set of neighbourhood for trading flows

$\hat{I}_t$ a set of all the passes i of technology t, except for the first pass of technology CF

C_t a set of contaminants processed by technology t

CF set of coagulation technologies with operating conditions within a given range

CLR clarification processes representative

CT_t a set of contaminants processed by technology t

I a set of water resources where $I = S \cup W$

I_t a set of passes and stages of technology t with a final pass, I_t^{max}

I_t a set of passes of technology t with a final pass, I_t^{max}

J_t a set of discrete levels for operating conditions of technology t

LW a set of land sources (sw, gw)

MF set of microfiltration technologies with operating conditions within a given range

MMF set of multi-media filtration technologies with operating conditions within a given range

ND a set of newly installed dams

NF set of nanofiltration technologies with operating conditions within a given range

NP a set of newly installed plants

OD a set of installed dams at the start of the planning time horizon

OP a set of installed plants at the start of the planning time horizon

PG_g a set of plants in a state g

$RO1$ set of reverse osmosis technologies with operating conditions within a given range to remove dissolved solids

$RO2$ set of coagulation technologies with operating conditions within a given range to remove boron

S a set of water sources (sw, gw, dw)

SP_i a set of plants treating a specific source s

$TCLR$ clarification processes SED and DAF

$TCLR$ clarification processes

TMM membrane processes

TMM membrane processes

$TMMB$ filtration processes

UF set of ultrafiltration technologies with operating conditions within a given range processes

W a set of water product (uw)

Parameters

$\bar{p}_{qj}$ operating pressure at discrete level j for technology q, [MPa]

$\bar{y}_{qis}$ recovery factor of technology q, pass i and stage s, [−]

$\bar{Y}_{si}$ recovery factor of technology s and pass i, [−]

$\epsilon_{i'ip}$ efficiency for plant p for source of water i' for production of product i, [−]

$\hat{Y}_{tisr}$ clarification technologies' recovery at discrete level r, [−]

λ_k parameter expressing the natural logarithm of reliability difference for an option k, [−]

μ viscosity of water source, $[kg/m \cdot s]$

μ viscosity of water source, [kg/m · s]

ξ_k parameter expressing the natural logarithm of cost difference for an option k, $[-]$

A_q parameter associated with the capital cost of technology q, [-]

A_t parameter associated with the capital cost of technology t, [-]

A_t parameter associated with the capital cost of technology t, [-]

af^{MCC} constant accounting for annualisation for equipment cleaning and maintenance, [-]

af^{MRC} constant accounting for annualisation for equipment replacement, $[-]$

af^{MRC} constant accounting for annualisation for equipment replacement, [-]

b_q parameter associated with the capital cost of technology q, [-]

b_t parameter associated with the capital cost of technology t, [-]

b_t parameter associated with the capital cost of technology t, [-]

c^{chem} coagulant price, [\$/t]

C^E electricity charge, $[\$/kWh]$

c^E electricity charge, [\$/kWh]

c_c^{IN} initial feed concentration of contaminant c, $[m^3/h]$

c_c^{IN} initial feed concentration of contaminant c, [mg/L]

C_{chem} coagulant price, $[\$/t]$

$capdam_l$ cost factors for building dams with capacity level l, $[bnUSD/GL]$

$capexp_{pl}$ cost factors for extending plant p with capacity level l, $[bnUSD/GL]$

$caplant_{pl}$ cost factors for building plant p with capacity level l, $[bnUSD/GL]$

cco_{tism}^{bp} capital cost at point m for unit belonging to technology t, pass i and stage s in piecewise linearisation, [\$]

cd_{tj} coagulant dose at discrete level j for technology t, [mg/L]

cdf_t capital costs discount factor, $[bnUSD/y]$

CO_{2_e} carbon dioxide equivalent, $[kg/kWh]$

CRF capital recovery factor, $[-]$

CRF capital recovery factor, $[-]$

cv^{CHC} a conversion constant for the chemical costs, $[-]$

cv^{CHC} a conversion factor for the coagulant costs, $[-]$

cv^{Ems} a conversion constant for the emissions taxes, $[-]$

cv^{EM} a conversion constant for the electrical mixing costs, $[-]$

cv^{EM} a conversion factor for the electrical mixing costs, $[-]$

cv^{PC} a conversion constant for the pumping costs, $[-]$

cv^{PC} a conversion factor for the pumping costs, $[-]$

cv^{SC} a conversion constant for the saturator costs, $[-]$

cv^{SC} a conversion factor for the saturator costs, $[-]$

D^{FM} fixed cost for downtime, [\$]

d_{tj}^{MED} media diameter of multi-stage media filtration at discrete level j for technology t, [m]

D^{VM} variable cost for downtime, [\$]

dct time for building a new dam, $[y]$

dem_{igtq} demand for a product w in region g at time t, $[GL/y]$

dff_g factor accounting for water distribution losses due to leakages in a region g, $[-]$

dsf factor for minimum reservoir storage, $[-]$

E^{max} maximum number of expansions, $[-]$

$ecap_{pl}$ expansion capacity of plant p for level l, $[GL/y]$

ect_p time for expanding a new plant p, $[y]$

ent_{igt} entitlements of water source i in a region g at time t, $[GL/y]$

eps epsilon values for ϵ-constraint solution approach, $[-]$

fop_{plt} fixed operating costs for plant p at capacity level l at time t, $[bnUSD/GL]$

gf_{tj} flocculation energy input at discrete level j for technology t, $[\mathrm{s}^{-1}]$

$icap_{pl}$ installation capacity of plant p for level l, $[GL/y]$

ict_p time for installing a new plant p, $[y]$

$idam_{glt}$ installation capacity of dam for level l in region g at time t, $[GL]$

$infl_q$ inflation rate for clarification technologies, $[-]$

$infl_t$ inflation rate, $[-]$

$infl_t$ inflation rate, $[-]$

ir interest rate, [-]

ir interest rate, [-]

L_{igtq} evaporation in a region g at times t and q, $[GL]$

l_{tj} length of the filter in multi-stage media filtration at discrete level j for technology t, [m]

$lc1$ constant associated with labour cost, [-]

$lc1$ constant associated with labour cost, [-]

$lc2$ constant associated with labour cost, [-]

$lc2$ constant associated with labour cost, [-]

ld_{tj} load to the multi-stage media filtration at discrete level j for technology t, [m/s]

LR^{ain}_{igtq} land rainfall in a region g at times t and q, $[GL]$

M big number, $[GL/y]$

M^{BIG}_c big number for contaminant c, [mg/L]

M^{CD} big number for coagulant cost, [\$/h]

M_c^{CONC} maximum allowable concentration of a contaminant c, [mg/L]

M_c^{CONC} maximum allowable concentration of a contaminant c, [mg/L]

M^{FLOW} minimum allowable final effluent from technology t, $[mg/L]$

M^{FLOW} minimum allowable final effluent from technology t, [m^3/h]

M^P big number for pumping pressure, [MPa]

M^{TG} big number for energy input and time, [−]

MC^O operating cost charge rate during maintenance, [−]

$mwco_{tj}$ molecular weight cut-off at discrete level j for technology t, [Da]

N^{max} maximum allowable number of passes, [-]

N^{MM} number of membrane modules, [−]

N_{max} maximum allowable number of passes, [-]

n_s number of shifts per day, [−]

$ocap_p$ installed capacity of plant p at the beginning of the planning horizon, $[GL/y]$

odf_t operating costs discount factor, $[bnUSD/y]$

$oldam_{gt}$ existing capacity of dams in region g at time t, $[GL]$

$oldplant_p$ existing capacity of plants, $[GL/y]$

p_{tj} operating pressure at discrete level j for technology t, [MPa]

pc penalty cost for not meeting urban water demand, $[bnUSD/GL]$

ph_{tj} hydrogen ion concentration at discrete level j for technology t, [-]

PY annual production yield, [-]

py annual production yield, [−]

Q^{IN} initial feed flowrate, $[m^3/h]$

Q^{IN} initial feed flowrate, [m^3/h]

q^{pbp}_{tism} product flowrate at point m for unit belonging to technology t, pass i and stage s in piecewise linearisation, [\$]

R^{ain}_{igtq} direct rainfall to storage in a region g at times t and q, $[GL]$

r^{ch} cost of treatment and post-treatment chemicals per volume of produced water, [\$/m^3]

r^{CO_2} carbon dioxide price, $[\$/kg]$

r^{infl} infiltration coefficient, $[-]$

R^{iver}_{igtq} streamflows in a region g at times t and q, $[GL]$

r^P pay rate per hour, $[\$/h]$

R^{unoff}_{igtq} runoff in a region g at times t and q, $[GL]$

R_{igtq} hydrological water inflows in a region g at times t and q, $[GL]$

r_{tcj} rejection coefficient of a contaminant c at discrete level j for technology t, $[-]$

RC^M replacement cost per module, [\$]

rc^M_t equipment replacement price for technology t per produced permeate, [\$/m^3]

rq_{tqcj} clarification technologies' rejection coefficients of a contaminant c at discrete level j, $[-]$

SP^{max}_{igt} maximum sustainable yield of source s in a region g at time t, $[GL/y]$

t_d number of operating days a year, [d/y]

t_d number of operating days a year, [d/y]

t_h number of operating hours a day, [h/d]

t_h number of operating hours a day, [h/d]

tem_{tj} operating temperature at discrete level j for technology t, [°C]

tf_{tj} flocculation time at discrete level j for technology t, [min]

trc_g selling transaction cost, $[bnUSD/GL]$

$trpr_{gtm}$ water selling price for region g at time t and option m, $[bnUSD/GL]$

U big number equal to the cardinality of the number of allowed passes, [-]

U_t^{BIG} big number for capital costs, [$]

up utilisation fraction of water which is collected and directed to wastewater treatment plants, $[-]$

vod_t variable cost factor for operating dams at time t, $[bnUSD/GL]$

vop_{plt} variable operating costs for plant p at capacity level l at time t, $[bnUSD/GL]$

WSR_{ig}^{min} minimum water reliability of region g, $[-]$

y_{tis} recovery factor of technology t, pass i and stage s, $[-]$

Y_{ti} recovery factor of technology t and pass i, $[-]$

yr years of investment, [-]

yr years of investment, [-]

η_t^{FP} pump efficiency, $[-]$

η_t^{FP} pump efficiency, [-]

η_t^{MT} motor efficiency, $[-]$

η_t^{MT} motor efficiency, [-]

η^{SAT} saturator efficiency, $[-]$

η^{SAT} saturator efficiency, [-]

π the ratio of a circle's circumference to its diameter, $[-]$

h_{tj} natural logarithm of component hydrophobicity at discrete level j for technology t, $[-]$

Binary variables

B_{igtq} binary variable equal to 1 in the year t and season q when supply exceeds demand, $[-]$

E_{gplt} binary variable equal to 1 if capacity level l of plant p in region g at time t is expanded, $[-]$

E_{tis} binary variable equal to 1 if technology t, pass i and stage s is selected, otherwise equal to 0, [−]

I_{gplt} binary variable equal to 1 if capacity level l of plant p in region g at time t is installed, [−]

ID_{glt} binary variable equal to 1 if capacity level l of dam in region g at time t is installed, [−]

W_{tisj} binary variable equal to 1 if level j of technology t, pass i and stage s is selected, otherwise equal to 0, [−]

W_{ti} binary variable equal to 1 if technology t and pass i is selected, otherwise equal to 0, [-]

WQ_{tqisj} binary variable equal to 1 if level j of technology q, pass i and stage s is selected, otherwise equal to 0, [−]

X_{qis} binary variable equal to 1 if technology q, pass i and stage s is selected, otherwise equal to 0, [−]

X_{si} binary variable equal to 1 if technology s and pass i is selected, otherwise equal to 0, [-]

Y^{m}_{tism} binary variable equal to 1 if position m of technology t, pass i and stage s is selected, otherwise equal to 0, [−]

Y_{gtm} binary variable equal to 1 if a price in a region g, time t and option m is selected, [−]

zc_{tisckl} binary variable equal to 1 if for technology t, pass i and stage s a number k and for power l is selected for concentrate, otherwise equal to 0, [−]

zf_{tisckl} binary variable equal to 1 if for technology t, pass i and stage s a number k and for power l is selected for feed, otherwise equal to 0, [−]

zo_{ckl} binary variable equal to 1 if a number k for power l is selected in effluent, otherwise equal to 0, [−]

zp_{tisckl} binary variable equal to 1 if for technology t, pass i and stage s a number k and for power l is selected for permeate, otherwise equal to 0, [−]

zr_{tisckz} binary variable equal to 1 if for technology t, pass i and stage s a number k and for power l is selected for separation efficiency and concentration disaggregation, otherwise equal to 0, [−]

zy_{tisr} binary variable equal for the reformulation of flowrate and recovery for clarification technologies, otherwise equal to 0, [−]

Integer variables

X_k an SOS type 2 variable equal to 1 if an option k for cost and reliability is selected, [−]

Continuous variables

$\bar{\tau}$ non-linear objective function for Nash bargaining approach, [−]

$C\bar{o}ut_{ck}$ auxiliary variable for effluent concentration for digit k, [mg/L]

$C\bar{R}^F_{tisck}$ auxiliary variable for feed concentration for technology t, pass i, stage s and digit k, [mg/L]

$\bar{C}^C_{tisck}$ auxiliary variable for concentrate concentration for technology t, pass i, stage s and digit k, [mg/L]

$\bar{C}^F_{tisck}$ auxiliary variable for feed concentration for technology t, pass i, stage s and digit k, [mg/L]

$\bar{C}^P_{tisck}$ auxiliary variable for permeate concentration for technology t, pass i, stage s and digit k, [mg/L]

$\bar{P}_{qis}$ operating pressure of unit q, pass i and stage s, [MPa]

$\bar{P}_{si}$ operating pressure of unit s and pass i, $[MPa]$

$\bar{Q}^F_{tisr}$ auxiliary variable for feed flow for technology t, pass i, stage s, [m^3/h]

$\bar{R}_{qisc}$ clarification technologies' rejection coefficients of a contaminant c in technology s and pass i, [−]

$\bar{R}_{sic}$ clarification technologies' rejection coefficients of a contaminant c in technology s and pass i, [−]

$\bar{Y}_{tis}$ recovery factor for CLR in MILFP model, [−]

$\bar{zc}_{tisck}$ continuous variable for disaggregation, [−]

$\bar{zf}_{tisck}$ continuous variable for disaggregation, [−]

$\bar{zo}_{ck}$ continuous variable for disaggregation, [−]

$\bar{zp}_{tisck}$ continuous variable for disaggregation [−]

$\bar{zr}_{tisck}$ continuous variable for disaggregation, [−]

$\hat{\tau}$ linear objective function for Nash bargaining approach, [−]

$C\hat{out}_{ckl}$ auxiliary variable for effluent concentration for digit k and point l, [mg/L]

$C\hat{R}^{F}_{tisckz}$ auxiliary variable for feed concentration for technology t, pass i, stage s, digit k and point z, [mg/L]

$\hat{C}^{C}_{tisckl}$ auxiliary variable for concentrate concentration for technology t, pass i, stage s, digit k and point l, [mg/L]

$\hat{C}^{F}_{tisckl}$ auxiliary variable for feed concentration for technology t, pass i, stage s, digit k and point l, [mg/L]

$\hat{C}^{P}_{tisckl}$ auxiliary variable for permeate concentration for technology t, pass i, stage s, digit k and point l, [mg/L]

$\hat{Q}_{igg'tqm}$ discrete traded flows of water i from a region g to a region g' at time t and q for option m, $[GL/y]$

A_{igtq} allocations of source i in region g at time t, $[GL/y]$

AC_{igtq} carry over for source s in region g at time t, $[GL/y]$

ACC total annualised capital cost, $[\$/yr]$

C^{C}_{tisc} concentrate concentration of contaminant c from technology t, pass i and stage s, [mg/L]

c^{F}_{tic} feed concentration of contaminant c to technology t and pass i, $[mg/L]$

C^{F}_{tisc} feed concentration of contaminant c to technology t, pass i and stage s, [mg/L]

c^{P}_{tic} permeate concentration of contaminant c from technology t and pass i, $[mg/L]$

C^P_{tisc} permeate concentration of contaminant c from technology t, pass i and stage s, [mg/L]

C^W_{tisc} concentration to waste of contaminant c from technology t, pass i and stage s, [mg/L]

$CAPEX_t$ total capital expenditure at time t, $[bnUSD/y]$

CC_{tis} capital cost for unit belonging to technology t, pass i and stage s, [$]

CC_{ti} capital cost for unit belonging to technology t and pass i, [$]

$CCol_{tis}$ capital cost for unit belonging to technology t, pass i and stage s in piecewise linearisation, [$]

CD_{tis} coagulant dose of technology t, pass i and stage s, [mg/L]

CD_{ti} coagulant dose, $[mg/L]$

$CDAM_t$ dams capital expenditure at time t, $[bnUSD/y]$

CHC chemical cost for technology t and pass i, $[\$/y]$

CHC_{tis} coagulant cost for technology t, pass i and stage s, [$/y]

$ChemC$ chemical cost for pH adjustment and post-treatment, [$/y]

$Cout_c$ final purity for contaminant c, [mg/L]

CPL_t plant capital expenditure for installation at time t, $[bnUSD/y]$

CQ^C_{tisc} continuous variable representing multiplication of concentrate concentrate and flowrate to a technology t, pass i and stage s, [g/h]

CQ^F_{tisc} continuous variable representing multiplication of feed concentration and flowrate to a technology t, pass i and stage s, [g/h]

CQ^P_{tisc} continuous variable representing multiplication of permeate concentration and flowrate from a technology t, pass i and stage s, [g/h]

$CQout_c$ continuous variable representing multiplication of concentrate concentrate and flowrate to a technology t, pass i and stage s, [g/h]

CR^F_{tisc} continuous variable representing multiplication of separation efficiency and concentration to a technology t, pass i and stage s, [mg/L]

D^{MED}_{tis} media diameter of multi-stage media filtration, [m]

D^{MED}_{ti} media diametre of multi-stage media filtration, $[m]$

D_{igtq} demand of a water source or end use i in a region g at time t, $[GL/y]$

DAM_{gt} capacity of dams in region g at time t, $[GL]$

DS_{igtq} dams storage of water i in a region g at times t and q, $[GL]$

EM mixing cost for technology t and pass i, $[\$/y]$

EMC_{tis} mixing cost for technology t, pass i and stage s, [$/y]

EMS_{ti} annual carbon emissions for technology t and pass i, $[kg/y]$

$EMSC$ emission charges for t and pass i, $[\$/y]$

G_{tism} continuous variable in piecewise approximation, $[-]$

Gf_{tis} flocculation energy input of technology t, pass i and stage s, [s^{-1}]

Gf_{ti} flocculation energy input, $[s^{-1}]$

L_{tis} length of the filter in multi-stage media filtration, [m]

L_{ti} length of the filter in multi-stage media filtration, $[m]$

LC labour cost, $[\$/y]$

LC labour cost, [$/y]

Ld_{tis} load to the multi-stage media filtration, [m/s]

Ld_{ti} load to the multi-stage media filtration, $[m/s]$

MCC cleaning and maintenance cost for technology t and pass i, $[\$/y]$

MRC replacement cost for technology t and pass i, $[\$/y]$

MRC_{tis} replacement cost for technology t, pass i and stage s, [$/y]

$MWCO_{tis}$ molecular weight cut-off for a membrane in technology t, pass i and stage s, [Da]

$MWCO_{ti}$ molecular weight cut-off for a membrane in technology t and pass i, $[Da]$

O_{igtq} outflow of water i in a region g at times t and q, $[GL]$

$ODAM_t$ dams operational expenditure at time t, $[bnUSD/y]$

$OPen_t$ penalty cost at time t, $[bnUSD/y]$

$OPEX_t$ total operational expenditure at time t, $[bnUSD/y]$

OPL_t plant operational expenditure at time t, $[bnUSD/y]$

OTR_t trading expenditure at time t, $[bnUSD/y]$

P_{igtq} production of a water source or end use i in a region g at time t, $[GL/y]$

P_{tis} operating pressure of unit t, pass i and stage s, [MPa]

P_{ti} operating pressure of unit t and pass i, $[MPa]$

PC pumping cost for technology t and pass i, $[\$/y]$

PC_{tis} pumping cost for technology t, pass i and stage s, [$/y]

PD_{igtq} penalty for unmet demand for source i, region g and time t, $[GL]$

pH_{tis} hydrogen ion concentration in feed to technology t, pass i and stage s, [-]

pH_{ti} hydrogen ion concentration in feed to technology t and pass i, [-]

PP_{tic} physicochemical properties of flow and operating conditions of technology t in pass i

PP_{tisc} physicochemical properties of flow and operating conditions of technology t in pass i and stage s, [-]

Q^{AP} annual production rate, $[m^3/y]$

Q^{AP} annual production rate, [m^3/y]

Q^{C}_{tis} concentrate flowrate from technology t, pass i and stage s, [m^3/h]

Q^{FL}_{tis} linearised feed flowrate and binary variable, [m^3/h]

Q^{F}_{tis} feed flowrate to a technology t, pass i and stage s, [m^3/h]

Q^F_{ti} feed flowrate to a technology t and pass i, $[m^3/h]$

Q^P_{tis} permeate flowrate from technology t, pass i and stage s, [m^3/h]

Q^P_{ti} permeate from technology t and pass i, $[m^3/h]$

Q^W_{tis} flowrate to waste from technology t, pass i and stage s, [m^3/h]

$Q_{igg'tq}$ traded flows of water i from a region g to a region g' at time t and q, $[GL/y]$

QCD_{tis} auxiliary variable to represent the multiplication of flowrate and coagulant dosage for a technology t, pass i and stage s, [g/h]

$Qout$ hourly capacity of the plant, [m^3/h]

QPf_{tis} auxiliary variable to represent the multiplication of flowrate and pressure for a technology t, pass i and stage s, [m^{3}MPa/h]

QtG_{tis} auxiliary variable to represent the multiplication of flowrate, flocculation energy input and time for a technology t, pass i and stage s, [m^3/h]

QY^F_{tis} continuous variable representing multiplication of feed flowrate and recovery to a technology t, pass i and stage s, [m^3/h]

R_{tic} rejection coefficient of a contaminant c in technology t and pass i, $[-]$

R_{tisc} rejection coefficient of a contaminant c in technology t, pass i and stage s, $[-]$

RC_{igtq} recharge of water i in a region g at times t and q, $[GL]$

SC operating cost for running the saturator in technology t and pass i, $[\$/y]$

SC_{tis} operating cost for running the saturator in technology t, pass i and stage s, [\$/y]

SS_{igtq} overall storage of water i in a region g at times t and q, $[GL]$

TC total annualised cost, $[\$/yr]$

TC total annualised cost, [\$/yr]

TC total capital and operating costs for the entire planning horizon, $[bnUSD]$

$TCAP_{gpt}$ capacity of plant p in region g at time t, $[GL/y]$

Tem_{tis} operating temperature for technology t, pass i and stage s, [°C]

Tem_{ti} operating temperature for technology t and pass i, [$°C$]

Tf_{tis} flocculation time of technology t, pass i and stage s, [min]

tf_{ti} flocculation time, [min]

trp_{gt} water selling price for region g at time t, [$bnUSD/GL$]

V_{igptq} plant intake of source s in region g in period t, [GL/y]

WNC water net cost, [$\$/m^3$]

WNC water net cost, [$\$/\mathrm{m}^3$]

WR total reliability of water supply, [$-$]

WS_{igtq} natural water storage i in a region g at times t and q, [GL]

WSR_{igtq} supply reliability of water i in a region g at times t and q, [$-$]

H_{tis} natural logarithm of component hydrophobicity of technology t, pass i and stage s, [$-$]

H_{ti} natural logarithm of component hydrophobicity influencing rejection in technology t and pass i, [$-$]

Chapter 1

Introduction

1.1 Global water outlook

Water is the most precious resource which sustains life by direct and virtual consumption, meaning through its embedment in clothes, food, electricity, etc. According to the United Nations, in the last century water demand has been increasing more than twofold than the population growth rate. By 2050, the world population is projected to reach 9.3 billion, out of which 70% will live in urbanised areas. As a result of the increment, food consumption will rise 60% from now. Furthermore, hydrological variability with climate change has profoundly been more ostensible through El Niño/ La Niña extreme weather oscillations. A combination of the aforementioned events have already contributed to a gap between supply and demand, which would exacerbate to hit 40% by 2030, and turn into seasonally severe water scarcity in the upcoming decades. Hence, improvements towards the efficient production and utilisation of the resource throughout the entire water cycle is crucial in order to address and mitigate water shortage [United Nations, 2016].

The water cycle (Fig. 1.1) begins with evaporation from and precipitation to lakes, rivers, groundwater and oceans. It is then stored and directed to surface water treatment, and groundwater and seawater desalination plants. Afterwards, it is distributed to agriculture, industry and household. Follows collection of sewerage, which is treated in wastewater treatment plants and safely returned back to their natural storage with which the cycle is completed.

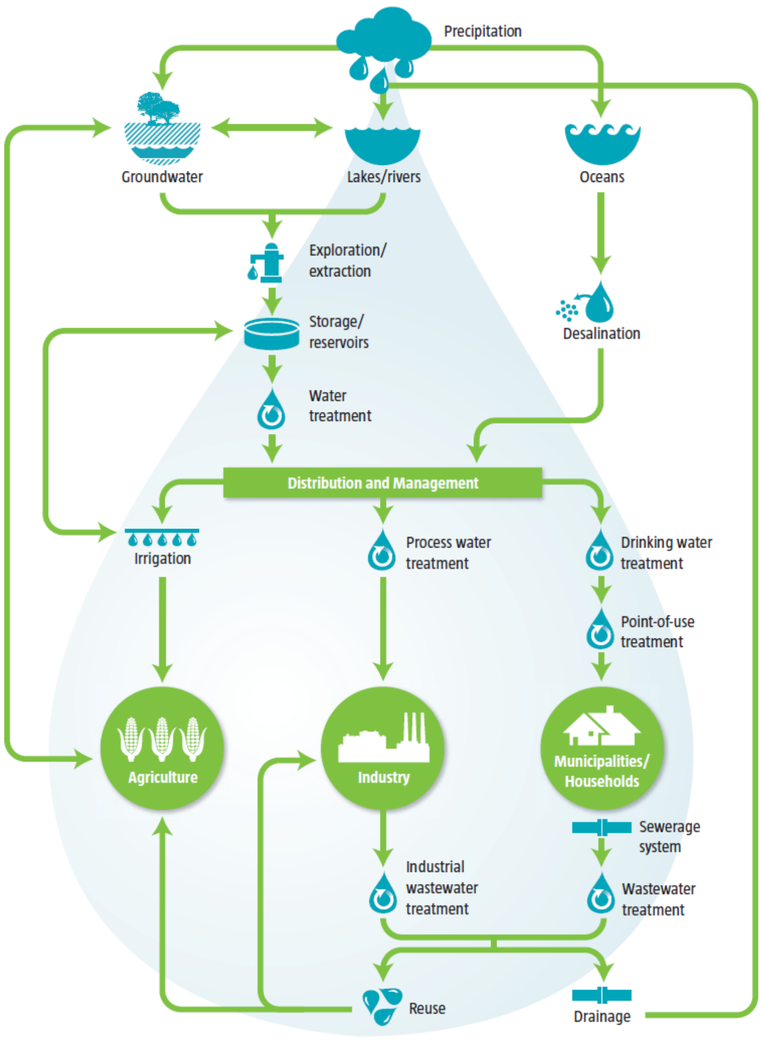


FIGURE 1.1: Water path from precipitation to usage
source: RobecoSam [2015]

Enhancements, therefore, can be performed at the points in the cycle where decisions are made of efficient water treatment and supply chain designs, which are recognised as a major solution to the arising burdens on world water resources [United Nations, 2012, British Petroleum, 2013, Chandrappa et al., 2011, Lior, 2013]. However, the processes still face challenges such as producing and distributing satisfactorily safe and affordable water [Hinkebein, 2004, National Centre of Excellence in Desalination Australia, 2011]. Examination of the economically viable purification paths and infrastructure planning at the early design stage can address those challenges [Barnicki and Siirola, 2005]. Taking a holistic approach at a project's conceptual design stage has the benefits of considering various aspects such as techno-economic, environmental and social domains, which can, consequently, assist water engineers, governments, institutions to make better informed decisions and policies. Often, considering the many miscellaneous components/options of a system, to select the most optimal one, can prove intricate due to the endless number of possibilities. Therefore, a systematic approach is required and mathematical modelling and optimisation theory are used as tools to tackle the complexity.

1.2 Optimisation techniques in water systems

Mathematical programming, or mathematical optimisation, is a powerful technique for identifying decisions which result in a maximisation/minimisation of an objective. There are four components to a mathematical programming model: variables, parameters, constraints and objective function, which are mathematically interconnected. The general structure of an optimisation problem is shown in Eq. (1.1), where $f(x, y)$ is the objective function, x and y are vectors of respectively n continuous variables and integer variables, $h(x, y)$ are equality and $g(x, y)$ inequality constraints [Floudas, 1999].

$$
\begin{aligned}
\min_{x,y} \;& f(x,y) \\
s.t. \;& h(x,y) = 0 \\
& g(x,y) \leq 0 \\
& \quad x \in X \subseteq R^n \\
& \quad y \in Y \;\; integer
\end{aligned}
\tag{1.1}
$$

Depending on the relationship between the variables in the constraints and objective function, models can be classified into the following categories [Nowatzki et al., 2013, Croce, 2013]:

- *Linear programming (LP)* models contain an objective, or objectives, which is a linear function of the variables and it is subject to linear equalities and inequalities.
- *Non-linear programming (NLP)* models with continuous variables and non-linearities either in the constraints or in the objective function, or in both.
- *Mixed integer programming (MIP)* models arise when a subset of the decision variables is constrained into solely integer values. When in an MIP all constraints and objective function are linear, it is referred to as a mixed integer linear programming (MILP), whereas if non-linear expressions are present, the models are

referred to as mixed integer non-linear programming (MINLP). A variation of the MINLP occurs when the non-linearity arises only from the objective function, being a quotient of two continuous variables. The type of programming is called mixed integer linear fractional programming (MILFP), which is tackled by solving iteratively a few MILP models.

In the last few decades, mathematical optimisation theory has advanced and currently, there are a number of fast commercial and academic solvers available. Such optimisers developed for linear programs are: CPLEX, GUROBI, MOSEK, SCIP, global solvers for non-linear programs are BARON, ANTIGONE, SCIP, and local solvers for non-linear programs are SBB, DICOPT, etc.. All the models in the thesis are implemented in General Algebraic Modelling System (GAMS) using a variety of the aforementioned solvers [Rosenthal, 2012]. Details are given in each chapter separately.

1.3 Overview of process synthesis

Definition

"The act of combining constituent elements of separate material or abstract entities into a single or unified entity."

Process, or Systems, Synthesis, as a systematic approach, is a research area originating in the 1970s. In the context of process synthesis, elements can refer to a technology or its component, and an entity can be a single technology or an entire flowsheet design. Two major types of approaches exist when it comes to process synthesis, i.e.: (i). seek to improve an existing flowsheet and (ii). determine an optimal flowsheet from scratch. The former case engages evolutionary methods and structural parameter methods as the initial solution already exists while the latter can be realised through breadth- and depth-first methods, bounding, heuristic and decomposition methods [Nishida et al., 2004].

Process design is carried out in a number of steps, illustrated in Fig. 1.2. Firstly, the most likely and feasible alternatives are identified from a pool of candidate technologies and interlinks. Together, they comprise the superstructure of possible units and connections, which contains the feasible sets of solutions. Out of the feasible set, a flowsheet is

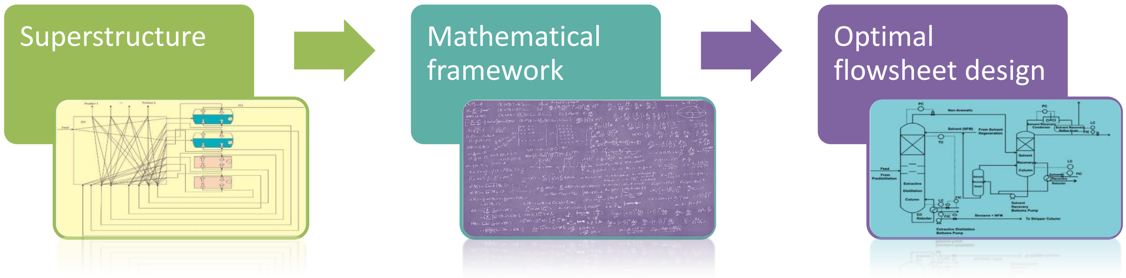


FIGURE 1.2: Steps in process synthesis

returned. A candidate is any possible technology configuration which is contained in the initial superstructure. Then, the evaluation criteria and tasks executions of technologies are represented in mathematical programming language. The most important objectives are identified as of whether it is sought to minimise cost, maximise throughput, minimise environmental impacts, maximise social wellness, etc. so as to meet qualitative and quantitative production targets set by industry, demand and environmental organisations. Due to modelling naturally non-linear systems, process synthesis problems are featured by MINLP representations [Floudas, 1999]. Finally, out of the given possibilities, one option is singled out which satisfies the given constraints and is an optimal or nearly optimal solution to the objectives required.

The process synthesis approach in this thesis uses superstructure optimisation and is formulated as an MINLP at first. As the complexity of the model architecture increases, approximation and linearisation techniques are applied to transform the problem into an MILFP model.

1.4 Overview of supply chains

Definition

"Entire network of entities, directly or indirectly interlinked and interdependent in serving the same consumer or customer. It comprises of vendors that supply raw material, producers who convert the material into products, warehouses that store, distribution centres that deliver to the retailers, and retailers who bring the product to the ultimate user. Supply chains underlie value-chains because, without them, no producer has the ability to give customers what they want, when and where they want, at the price they want. Producers compete with each other only through their supply chains, and no degree of improvement at the producer's end can make up for the deficiencies in a supply chain which reduce the producer's ability to compete."

Entities may refer to any stage of the supply chain (SC), i.e. manufacturers, suppliers, retailers and customers, from raw materials to distribution of a final product [Sousa et al., 2007, Sung and Maravelias, 2007]. The flow of materials in supply chain goes from manufacturers to consumers and is driven by the resources availability and supply, while the information of demand flows in the opposite direction. General supply chain structure and supply-demand relationship are illustrated in Fig. 1.3.

Supply chain planning occurs at three different hierarchical levels, namely, long-term, mid-term and short-term level. Long-term planning involves the strategic supply chains network design, from beginning to end. In this level, key infrastructure decisions are made as of where and when to invest in building a warehouse, plant, distribution centre or transportation system. Typically, the planning horizon takes years and takes into account projections in demand. Next, mid-term supply chain levels deal with master and demand planning. The planning horizon can be in the order of months. Finally, short-term design is executed in a matter of hours and days in order to deal with purchasing, production planning and scheduling, distribution and transport organisation and demand fulfilment [Voßand Woodruff, 2006]. The objective in supply chain design, depending on hierarchical level, is to minimise cost, stock-out probability, product demand variance, maximise profit, available system capacity, or achieve target service level, etc..

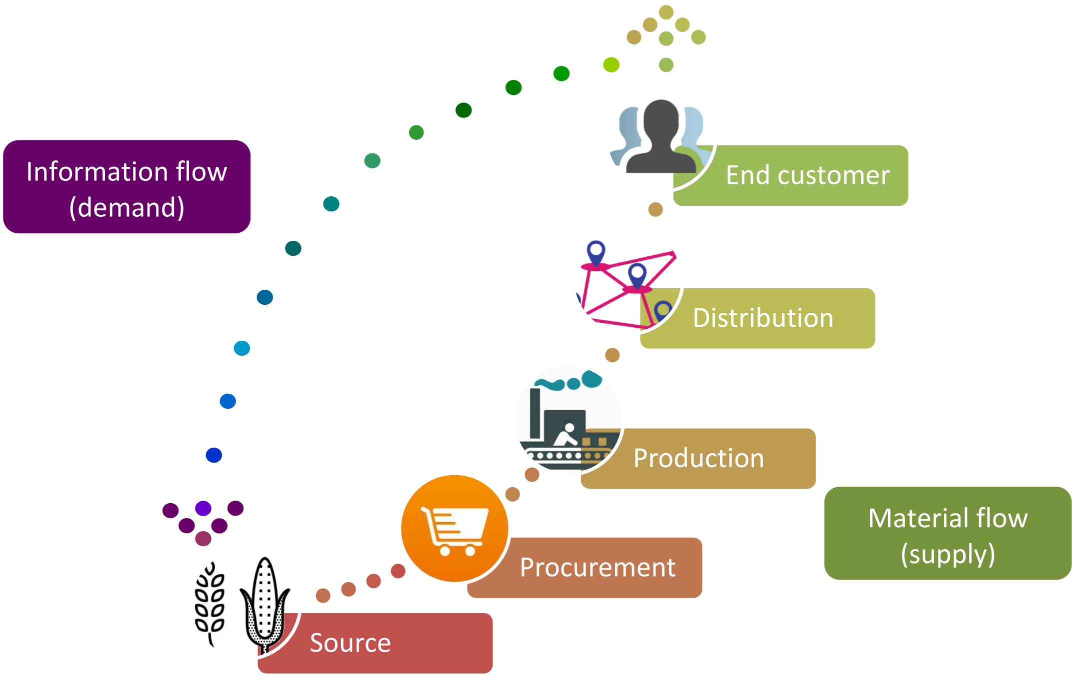


FIGURE 1.3: Supply chain structure, material and information flow

The supply system framework in this thesis entails long-term strategic level decisions for water supply systems, such as infrastructure and capacity expansion, which is implemented through an MILP formulation.

1.5 Thesis aim

To address the issued discussed earlier, this thesis aims to develop interdisciplinary approaches for the design and planning of different scales of water systems in order to assist water engineers and policy makers in decision processes. The research contributions by topic are listed below:

- *Conceptual Water Treatment Flowsheet Design*
  An MINLP and an MILFP frameworks are proposed where (i) unique superstructure accommodating the technologies widely integrated across water and advanced wastewater treatment, and desalination is developed; this allows to flexibly apply the problem in various water industries through including the relevant contaminants found in the water source; (ii) removal efficiencies are modelled as continuous variables as a function of the operating conditions of the candidate technologies;

this allows identifying the optimal operating conditions of every unit on the flowsheet. Flowsheet can be referred to as a process flow diagram where only the major plants' units their connectivity are depicted.; (iii) operating costs breakdowns and capital costs for every candidate technology are featured; this allows for more accurate conceptual design production cost estimation.

- *Water Supply System Design and Planning*
  An MILP framework for water supply system is developed which combines (i) climatic change through hydrological modelling, (ii) resources allocation, (iii) trading schemes and pricing collectively.

- *Multi-objective Supply System Optimisation*
  A multi-objective MILP framework is designed for the minimisation of supply system infrastructure cost and the maximisation of reliability of supply throughout the planning horizon using two approaches.

1.6 Thesis outline

The remaining work in the thesis is organised in five chapters in an ascending order of design scale, starting from the smallest system.

Chapter 2 presents a mathematical framework for the synthesis of water and water-related treatment processes for the production of water at desired purity at minimum overall cost. The optimisation problem is formulated as an MINLP model. A general superstructure is proposed, which incorporates the most common commercial technologies and the major pollution indicators, such as total suspended solids (TSS) and total dissolved solids (TDS). The model is tested on two case studies, i.e. seawater desalination and tertiary wastewater treatment. The results are analysed and compared to existing guidelines in order to examine the applicability of the proposed approach.

Chapter 3 builds further on Chapter 2 by introducing new elements to the problem superstructure. Due to the model's numerous non-linearities and consequently, its non-stability, various linearisation, approximation and reformulation techniques are implemented. Consequently, two improved formulations are derived, i.e. a partially linearised MINLP (plMINLP) and a mixed integer linear fractional programming (MILFP) models.

The applicability of the mathematical formulations are investigated in case studies of seawater desalination and surface water treatment for the production of potable water. Finally, the models performance is analysed and compared against each other.

In Chapter 4 an optimisation approach is developed and formulated as a spatially-explicit multi-period Mixed Integer Linear Programming (MILP) model, for the design of water supply system at regional and national scales. Assessment of available resources for withdrawal is performed based on hydrological balances, governmental rules and sustainable limits. Surface water, groundwater, and seawater are considered, which can be treated in different purification plants located in disparate regions in a country. The optimisation framework encompasses decisions such as installation of new purification plants, capacity expansion, and raw water trading schemes. The objective is to minimise the total cost incurring from capital and operating expenditures.

Chapter 5 extends the mathematical problem in Chapter 4 to a multi-objective framework. In the light of the increasing importance of reliability of water supply, a second objective, seeking to maximise the reliability of the supply system, is introduced. The ϵ-constraint method and Nash bargaining approach are used as solution methods to the multi-objective formulation. The former provides the possible optimal solutions for design while the latter identified the optimal Pareto solution at equilibrium. The capability of the models are addressed through a case study about Australia. The frameworks can assist local governments in the decision making for the water supply infrastructure of the country.

In Chapter 6 the contributions of this work are summarised, major concluding remarks are drawn and potential future work is suggested.

Part I

Design and Optimisation of Water Treatment Processes

Chapter 2

Synthesis of Water Treatment Processes with Passes

This chapter aims at developing an optimisation framework for water and water-related treatment flowsheet design considering a pool of various candidate technologies.

2.1 Theoretical Background

World water baseline scenario for year 2050 reveals approximately $5,500\,km^3$ of freshwater withdrawals will be required to meet the demand of water necessary for manufacturing, electricity production and domestic use. This represents an increase of 55% from current global demand where 130% more drinking water will be in demand for households than volumes nowadays [United Nations, 2015].
Water supply to end users is governed by publicly accepted practices which entail sources such as groundwater or surface water to undergo water treatment. Seawater desalination has become an alternative option for the provision of clean water. After purification, the product water is distributed to agriculture, industry and households. The connecting domain in the water supply chain belongs to water treatment and desalination. Hence, with the outlook of future water demand, investments on new purification plants have been planned. By 2018, for instance, Middle East and Africa are expected to have an annual growth of water production capacity of 13.2%, followed by Asia with 10.1% and the Americas with 5.7% (Fig. 2.1). Desalination, on the other hand, has gained popular-

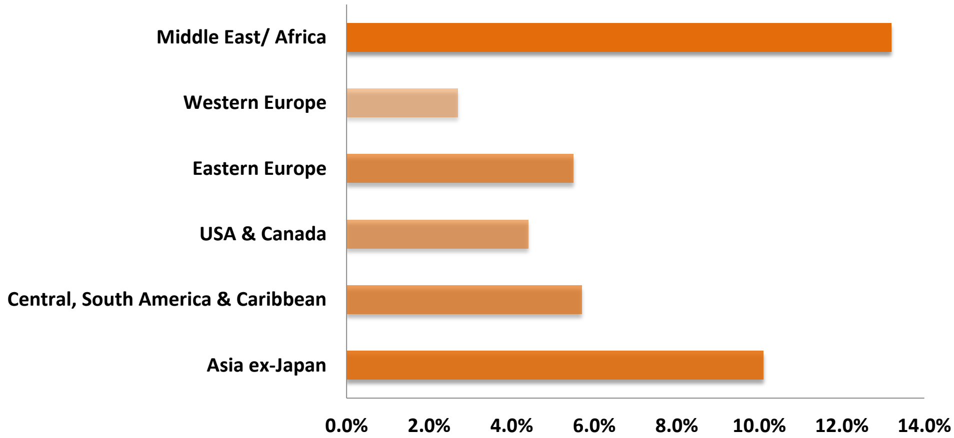


FIGURE 2.1: Projected percentage of increase of water utilities by area by 2018
source: RobecoSam [2015]

ity in less than a century. It has evolved from an idea in 1951 into an industrial process with large clean water production capabilities today. Fig. 2.2 depicts the progressively installed desalination plants capacities in selected countries from the discovery of reverse osmosis to 2016. The global desalination capacity by the end of 2016 is projected to

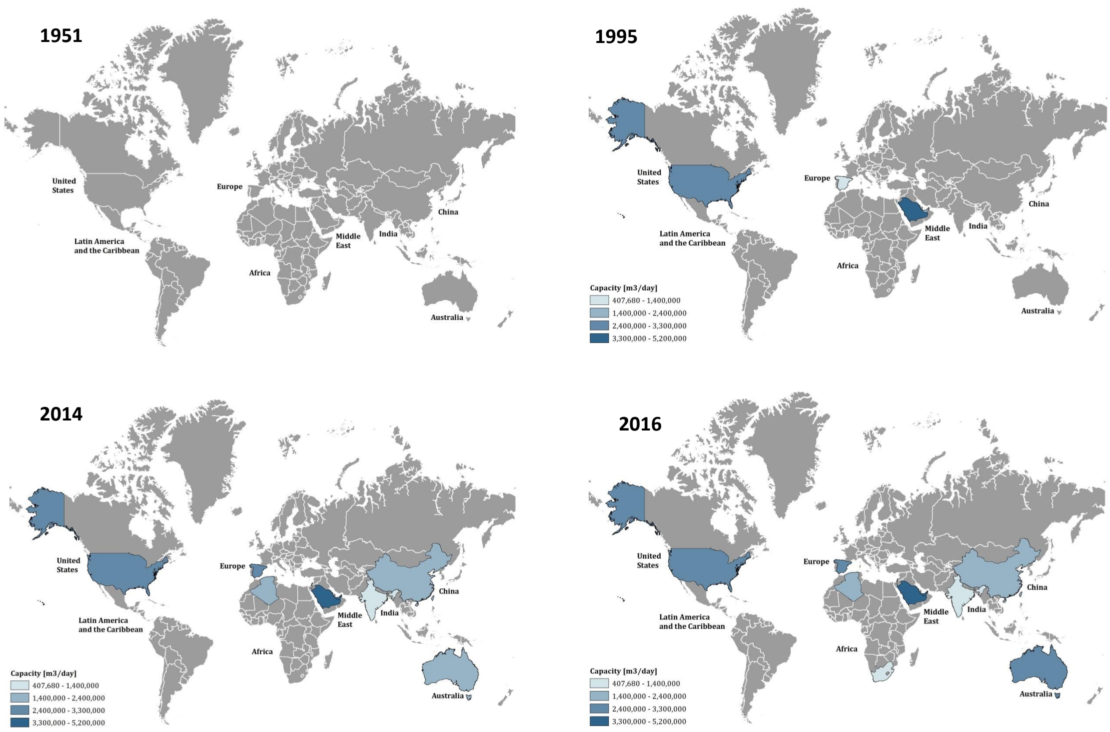


FIGURE 2.2: Progress of top 10 countries - leaders in desalination
source: Pacific Institute [2013], DesalData [2014], Global Water Intelligence [2016]

be 86.8 million m^3 which is predicted to reach 128 million m^3 by 2018 [International

Desalination Association, 2016].

Therefore, there is an increasing interest in developing systematic methods for optimising water separation units together with their interconnections [Nishida et al., 2004]. The selection of water technologies, process units and their sequence depends on the influent and effluent characteristics, nature of contaminants and treatment cost [Tchobanoglous et al., 2003]. Based on those attributes, water treatment can be classified into a number of applications, such as brackish and seawater desalination, and water and wastewater treatment.

Amongst the existing desalination technologies developed in the last decades, thermal (conventional) and membrane (non-conventional) desalination methods take the upper hand in large-scale plants. The conventional methods are represented by multi-stage flash (MSF), multi-effect distillation (MED) and vapour compression (VP), whereas the commercially available membrane technologies include nanofiltration (NF), reverse osmosis (RO) and electrodialysis (ED) [Afify, 2010]. The selection between conventional and non-conventional treatment depends on technical, economic and geographical attributes [Vince et al., 2007]. Water plants, deploying thermal technologies, exhibit high purification efficiencies, but at the expense of high energy requirements and therefore, not economically viable when not coupled with a power plant. Membrane plants, however, exhibit economic and environmental advantages over thermal plants [Sassi and Mujtaba, 2010]. Pressure and vacuum-driven membrane processes, in particular, are preferred because of their efficiency and no need of fluid phase change [Chan and Tsao, 2003]. Further, pretreatment technologies are also divided into conventional and non-conventional. The former group is represented by coagulation-flocculation (CF), sedimentation (SED), dissolved air flotation (DAF) and granular or multi-media filtration (MMF), and the latter encompasses microfiltration (MF) and ultrafiltration (UF). Over the last decade, membrane pretreatment technologies have advanced significantly and today they accommodate lower footprint, constant permeate quality in cases of algal blooms, higher retention of organics and reduced chemical consumption [Wilf and Schierach, 2001, Wilf et al., 2007, Villacorte, 2014]. Fig. 2.3 presents recent statistics where more than half of the world desalination plant capacities are operated on the principle of MF/UF for pretreatment and NF/RO for desalting [Villacorte, 2014].

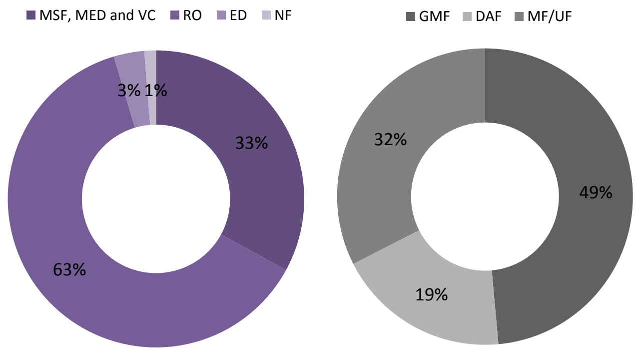


FIGURE 2.3: Global installed capacity for pretreatment (right) and desalting (left) by technologies

adapted from: Villacorte [2014]

When inorganic and some organic wastes are treated in wastewater during advanced wastewater treatment, and when contaminants from surface or ground water are removed, physico-chemical process units predominate. Such technologies are coagulation - flocculation (CF), sedimentation (SED), dissolved air flotation (DAF), media and membrane filters, ion exchange and carbon adsorption units [Forster, 2003, Cheremisinoff, 2002, Tchobanoglous et al., 2003]. As the technologies for the major water purification applications coincide, it can, therefore, be possible to develop an approach, followed by a mathematical model, for the synthesis and optimisation of flowsheets taking into account the aforementioned water sources and technologies. From now on the authors would refer to a collective term of all the purification applications solely as water treatment processes.

Numerous works have been published on the design and optimisation of units and processes from water treatment applications. Voutchkov [2013] and Lior [2013] reviewed overall design of seawater desalination processes. Non-linear program and mixed integer non-linear program models have been proposed for the design and optimisation of MSF, MED, hybrid MED-RO and RO networks by Mussati et al. [2001], Druetta et al. [2013], Skiborowski et al. [2012], Sassi and Mujtaba [2013], Ruiz-Saavedra et al. [2014]. Spiller et al. [2015], Avramenko et al. [2004], Tchobanoglous et al. [2003], Cheremisinoff [2002] published guidelines for the design of water and wastewater treatment plants. Roberts and Inniss [2014] experimentally determined the link between source water quality and treatment sequence. Franceschi et al. [2002] and Rossini et al. [1999] investigated the optimal operation of coagulation-flocculation to handle raw water qualities by numerical methods, taking an iterative approach. Mixed Integer Non-Linear Program (MINLP) methods for the synthesis of water and wastewater networks were also considered in some works [Galán and Grossmann, 2011, Ibrić et al., 2014]. Sweetapple et al. [2014] suggested a multi-objective optimisation of wastewater treatment plant to minimise the operating cost, greenhouse gas emissions and effluent contaminants concentrations. The economic appraisal of systems as an essential part of optimisation has been discussed in various publications. For instance, Pickering and Wiesner [1993] proposed a cost model for low pressure membrane filtration, Wright and Woods [1993] developed a capital cost correlation for UF units, whereas Fuqua et al. [1991] published a method for the estimation of RO units. Additionally, Lu et al. Lu et al. [2006] suggested an MINLP cost model for RO systems in desalination processes with focus on pumping, and membrane cleaning and replacement. Later a model with multiple feed and multiple product to minimise the total annual cost of the system was introduced [Lu et al., 2012]. A global strategy for the estimation of water production cost in water and wastewater treatment plants was presented by Kumar et al. [2015]. Large scale RO network cost minimisiation was performed in the work of Jiang et al. [2015] and multi-objective MINLP models for annaulised cost and energy consumption were presented in the works of Du et al. [2014] and Vince et al. [2008].

In some of those works, a holistic synthesis and optimisation of wastewater treatment with single and multiple contaminants have been proposed [Tsiakis and Papageorgiou, 2005, Skiborowski et al., 2012, Gabriel et al., 2015, Teles et al., 2012, Khor et al., 2012a]. Deterministic design of water, wastewater and seawater treatment processes formulated as non-linear programming (NLP) or mixed integer non-linear programming (MINLP) models has been studied in various works [Khor et al., 2012a, Teles et al., 2012, Sueviriyapan et al., 2016, Koleva et al., 2016a]. Multi-objective optimisation for minimising operating costs, greenhouse gas emissions and effluent contaminants has been presented by Sweetapple et al. [2014].

Water network systems (WNS) together with wastewater treatment have been the focus of copious articles [Tokos and Pintarich, 2009, Khor et al., 2012b, Dong et al., 2008, Ahmetović and Grossmann, 2011, Galán and Grossmann, 2011, Rojas-Torres et al., 2013, Ibrić et al., 2014, Yang and Grossmann, 2013]. A recent comprehensive review analysed and classified the various contributions made to WNS [Ahmetović et al., 2015]. Integrated water resources management studies have taken into account different water and wastewater treatment options formulated as single and multi-objective optimisation problems [Liu et al., 2010, 2011, Liu and Papageorgiou, 2013]. Guerra et al. [2016a] have presented a novel method for the design of shale gas supply chain with wastewater management where total dissolved solids are considered.

Definition

"Water network systems (WNS) can be defined a set of water treatment units and interconnections which can exist as a secondary system in a chemical plant or a stand-alone treatment plant."

Despite the extensive work done on modelling and optimisation of water treatment units and networks, general methodologies focusing on the optimal design of a range of water and water-related purification processes seek more research attention. This is particularly relevant when optimising the performance of individual technologies for the development of an entire flowsheet.

The present work addresses the gap by presenting a systematic approach for the design of water treatment processes, with a particular focus on surface water and advanced wastewater treatment, and brackish and seawater desalination. The problem is formulated as a mixed integer non-linear programming (MINLP) model. The rest of the chapter is organised as follows: Section 2.2 outlines the scope of the problem, followed by the presentation of the mathematical model in Section 2.3. Next, two theoretical case studies are looked at, together with results, computational performance and discussion in Section 2.4 and Section 2.5. Finally, the main conclusions are drawn and further work directions are suggested in Section 2.6.

2.2 Problem statement

The aim of the current work is to develop a methodology for the generation of a combination of technologies and number of passes that result in the most economically favourable flowsheet design. The proposed model involves 4 major groups of contaminants, i.e. chemical oxygen demand (COD), dissolved organic carbon (DOC), total suspended solids (TSS) and total dissolved solids (TDS). The presence of Boron (B), which is classified as part of the TDS group, requires special considerations, consequently, it

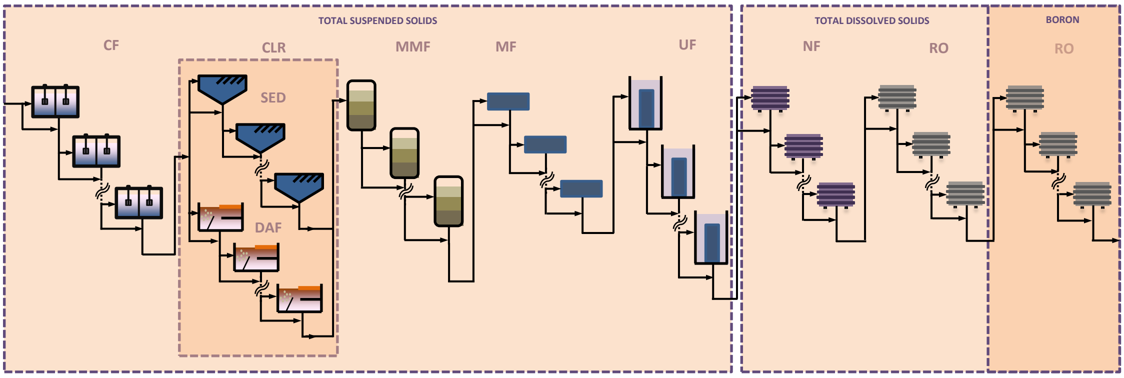


FIGURE 2.4: Superstructure of the proposed model

is considered separately. The technology candidates studied are 9, namely, coagulation-flocculation (CF), sedimentation (SED), dissolved air flotation (DAF), multi-stage media filtration (MMF), microfiltration (MF), ultrafiltration (UF), nanofiltration (NF), reverse osmosis (RO) for TDS (RO1) and B (RO2) removal. A model superstructure including all acceptable technology options and connections is presented in Fig. 2.4. The dashed line boxes represent the blocks of equipment that are associated with the removal of a group of contaminants. For instance, CF, SED, DAF, MMF, MF and UF remove the suspended solids, whereas NF removes the dissolved solids, and RO removes both, dissolved solids and boron. It is assumed that organic matter can be removed by conventional treatment such as CF, smaller pore – size low filtration membranes, such as UF, and larger pore – size high pressure membrane, such as NF. MMF does not exhibit a molecular weight cut – off for organics, and irreversible fouling is observed on RO membranes, hence, not used for that particular application.

General heuristics that apply to process synthesis advise removal of unstable materials early, separate most abundant components at first and leave the sturdiest operation for last [Rousseau, 1987]. In this case, suspended solids can be exposed to shear stresses, break up and consequently, clog the equipment which justifies its removal at first. TDS is the most plentiful contaminant and boron is difficult to separate from water, which assigns them a second and third place in the separation sequence, respectively. Filtration processes units decrease in their molecular weight cut-off, or pore size, from left to right in the above figure in order to prevent fouling.

Having defined the separation requirements, the sequence of the technology candidates in the model is pre-fixed. The water engineering industry practices used for the construction of the superstructure eliminate the possibility of backward flow. A candidate, however, can be either selected or bypassed. In the majority of cases, coagulation-flocculation requires a clarification process downstream. Two clarification options are provided, SED and DAF, represented by the collective name CLR. If any of those two processes is selected, a clarification process is selected, too. Whenever a clarification process is chosen, the selection of CF is mandatory. On its own, CF can be selected if the separation is efficient enough. In the current work, the filtration processes are allowed to exist in the flowsheet sequentially, although it is possible to restrict the problem to the selection of one low pressure membrane process, i.e. MF or UF, and one high pressure membrane process, i.e. NF and RO. The decision whether a pass from a technology is singled out or not is represented by one binary variable and as many passes as desired can be assigned to a technology. A pass, denoted by i, refers to the sequential repetition of a technology. A pass is used in order to increase product purity. The selection of the technologies is based on meeting the regulatory requirements for water plant effluent [The Drinking Water Inspectorate, 2009, U.S. Environmental Protection Agency, 2010] and minimising the water net cost, expressed in US$/m^3. For modelling purposes, the following simplifications and assumptions were made:

Assumptions

- rejection coefficients and recoveries are the major technological performance criteria
- modified regression models return a reliable estimation for the rejection coefficients
- TDS, TSS and boron are the only contaminant indicators in seawater source whereas COD, DOC, TDS and TSS are the contaminants assumed to be present in secondary wastewater effluent
- the removal of a non-targeted group of contaminants from a particular technology is considered insignificant
- the selection of initial removal grids and intake screens are not taken into account in design
- complete recovery of microfiltration and ultrafiltration filters
- no fouling and flux decrease take place and therefore, the observed phenomena as a result of those do not apply. This implies removal efficiencies will remain constant between cleaning cycles due to the absent pressure build.
- no system pressure losses
- replacement and cleaning costing for RO is assumed to apply for MF, UF and NF
- there are 65 days allocated for major maintenance, i.e. plant shut down
- social, political and geographical dimensions are excluded from the cost model
- annual water production and operating expenses remain the same throughout the plant's commercial lifespan
- no government incentives for the construction and commission of the water treatment facilities is considered
- MWCO, hydrophobicity and pH do not affect membranes' operating costs directly
- governments do not tax carbon emissions of water treatment plants

The overall optimisation problem is stated below.

Given:

- major constituent contaminants in source water
- pool of water treatment technologies
- a number of passes, or sequential units, from a technology
- source water intake flowrate
- key parameters of source water contaminants (e.g. initial concentrations) and key parameters for treatment technologies (e.g. recoveries, saturator, pump and motor efficiencies)
- candidate technologies characteristics ranges (e.g. flocculation time and energy input, coagulant concentrations, operating pressures, influent temperature, hydrophobicity, hydrogen ion concentrations, molecular weight cut - offs)
- cost data (e.g. units upfront costs, chemicals and electricity charges, maintenance and replacement rates, carbon tax rate, work pay rate, interest rate and plant life)

Determine:

- process flowsheet including multiple-pass strategy
- optimal operating conditions for the selected units
- contaminants and flowrates profiles
- annual operating and capital costs

So as to:

minimise the water production cost which equals the total annualised cost divided by the annual production rate.

2.3 Mathematical formulation

2.3.1 Performance criteria

The main performance criteria for water technologies are based on the purification standards and productivity that have to be achieved. These depend on the extent to which they reject major contaminants under specific set of conditions, and to which the product volumetric flowrate is recovered from the process.

2.3.1.1 Rejection coefficient

For any separation process, contaminant removal efficiency classifies as an essential performance criterion [Judd and Jefferson, 2003] because it guarantees a product meets its design purity specifications. The removal efficiency of downstream water purification processes can be measured by removal, rejection, retention or deactivation coefficient as a function of the contaminants physicochemical properties ($\mathrm{PP_{tic}}$) (2.1) such as coagulant concentration, headloss, filtration media dimensions, molecular weight, hydrophobicity, feed temperature, pressure and concentration, technology characteristics, etc [Benjamin and Lawler, 2013, Scott and Hughes, 1996, Xu et al., 2005]. It can take values between 0 and 1 as the former refers to no separation from a targeted contaminant and the latter refers to 100% separation achieved.

$$R_{tic} = f(PP_{tic}) = 1 - \frac{c^P_{tic}}{c^F_{tic}}, \qquad \forall t, i \in I_t, c \in C_t \tag{2.1}$$

where c^P_{tic} and c^F_{tic} are the concentrations of contaminant c in permeate and feed, respectively, associated with a technology, t, and its pass, i. The removal efficiencies following are represented in the form of regression models based on Analysis of Variance (ANOVA) for each of the considered processes.

The coagulation – flocculation treatment stage removes organic matter under the form of chemical oxygen demand (COD) and dissolved organic carbon (DOC), expressed in the constraints below, developed from findings in literature [Sangeetha et al., 2014, Park et al., 2000].

$$R_{tic} = 0.00058 \cdot CD_{ti} + 0.135 \cdot pH_{ti} - 0.154, \qquad \forall t \in CF,\ i \in I_t,\ c \in COD \tag{2.2}$$

$$\begin{aligned} R_{tic} =& 0.046 \cdot CD_{ti} + 2.915 \cdot pH_{ti} - 0.0003 \cdot CD^2_{ti} - 0.002 \cdot CD_{ti} \cdot pH_{ti} - \\ & 0.235 \cdot pH^2_{ti} - 9.486, \ \ \forall t \in CF,\ i \in I_t,\ c \in DOC \end{aligned} \tag{2.3}$$

where CD_{ti} and pH_{ti} are the coagulant dose and the hydrogen ion concentration for liquid in pass i from technology t. In the presence of organic matter, in literature this step is referred to as enhanced coagulation, which for simplification purposes, is going to be called CF in this work.

In the current model it is assumed the rejection of contaminants occurs at the clarification stage, i.e. sedimentation or dissolved air flotation. This means that rejection coefficients in the conventional candidates will be affected by the performance of the coagulation-flocculation process. Vlaški [1998] investigated experimentally the removal efficiency of sedimentation and dissolved air flotation depending on the operating characteristics of the typically preceding coagulation-flocculation process. If a clarification technology, CLR, is selected either SED's or DAF's rejection coefficient, $\bar{R}_{sic}$, will be valid (Eq.(2.4)).

$$R_{tic} = \sum_{s \in TCLR} \bar{R}_{sic} \cdot X_{si}, \qquad \forall t \in CLR,\, i \in I_t,\, c \in TSS \tag{2.4}$$

where X_{si} is a binary variable denoting the selection of a clarification technology or not. It has been then reported that sedimentation is strongly influenced by coagulant dose. After performing a regression analysis on the data provided in Vlaški [1998], the following equation has been obtained:

$$\bar{R}_{sic} = 0.22154 + 0.02516 \cdot CD_{ti}, \qquad \forall s \in SED,\, t \in CF,\, i \in I_t,\, c \in TSS \tag{2.5}$$

where CD_{ti} is the amount of coagulant used in the coagulation - flocculation process. DAF, showed dependence not only on the coagulant dose but also on the detention time and velocity gradient, denoted as tf_{ti} and Df_{ti}, respectively, in Eq.(2.6).

$$\begin{aligned} &\bar{R}_{sic} = 1.85886 - 0.00807 \cdot CD_{ti} - 0.00083 \cdot Gf_{ti} + 0.0025 \cdot tf_{ti} - 2.47 \cdot P_{si}, \\ &\qquad \forall s \in DAF,\, t \in CF,\, i \in I_t,\, c \in TSS \end{aligned} \tag{2.6}$$

where P_{si} is the pressure of the saturator.

A model developed by The Commonwealth Scientific and Industrial Research Organisation (CSIRO) predicted the initial steady-state removal of TSS in multi-stage media filtration (MMF) [Lin et al., 2006]. The relationship is shown in Eq.(2.7).

$$\begin{aligned} &R_{tic} = 0.0298 \cdot D_{ti}^{MED} + 0.171 \cdot Ld_{ti} + 0.206 \cdot L_{ti}^{-1} - 0.245, \\ &\qquad \forall t \in MMF,\, i \in I_t,\, c \in TSS \end{aligned} \tag{2.7}$$

where D_{ti}^{MED} designates the diametre of the media, Ld_{ti} is the load to the filtration process, L_{ti}^{-1} is the length of the filter for MMF and pass i.

The separation efficiency of TSS from water by MF is shown in Eq.(2.8) derived from experimental work [Benitez et al., 2006].

$$R_{tic} = 0.126 + 0.001 \cdot Tem_{ti} + 0.97 \cdot P_{ti}, \qquad \forall t \in MF,\ i \in I_t,\ c \in TSS \tag{2.8}$$

where Tem_{ti} is the temperature of the influent to technology t and pass i, and P_{ti} is the pressure of the feed flowrate. Besides TSS, in the work is reported the separation efficiency of MF from COD, expressed in Eq.(2.9).

$$R_{tic} = 0.189 + 1.09\ \cdot\ P_{ti}, \qquad \forall t \in MF, i \in I_t, c \in COD \tag{2.9}$$

For the removal of turbidity by UF, Eq.(2.10) holds.

$$R_{tic} = 0.959 - 1.510 \cdot P_{ti}, \qquad \forall t \in UF,\ i \in I_t,\ c \in TSS \tag{2.10}$$

where the equation has been derived from data obtained from pilot plant experimental work. It has been reported that turbidity and total suspended solids are related [Gallegos, 1993]. Hence, Eq.(2.10) can give an approximate estimation of the suspended solids removal in water treatment. The removal characteristics of UF embrace the reduction of COD and DOC, shown in Eq.(2.9) and Eq.(2.12) [Benitez et al., 2006, J. Cho and Pellegrino, 1999].

$$R_{tic} = 0.236 - 0.952 \cdot P_{ti}, \qquad \forall t \in UF,\ i \in I_t,\ c \in COD \tag{2.11}$$

$$R_{tic} = 1.224 - 0.00011 \cdot MWCO_{ti} + 0.79\ \cdot\ P_{ti}, \qquad \forall t \in UF,\ i \in I_t,\ c \in DOC \tag{2.12}$$

where $MWCO_{ti}$ is the molecular weight cut-off in Daltons. The performance characteristics of nanofiltration membranes are affected by solute properties, solution pH and membrane characteristics such as pore size, hydrophobicity and surface roughness [Artug, 2007]. Hence, the retention of dissolved uncharged organic compounds for NF can be approximated using contaminants hydrophobicity and molecular weight cut - off. The relation has been reported in literature based on laboratory experiments [Boussu et al., 2008].

$$R_{tic} = (0.57 - 0.07 \cdot H_{ti} - 0.0002 \cdot MWCO_{ti})^2, \qquad \forall t \in NF,\ i \in I_t,\ c \in TDS \tag{2.13}$$

where H_{ti} is the common logarithm of the unit's hydrophobicity. Eq. (2.14) and Eq.(2.15) show the retention of COD and DOC, respectively, where both coefficients depend on the membrane molecular weight cut-off and pressure [M. Tokhy and Bazedi, 2013].

$$R_{tic} = 1.138 - 0.00096 \cdot MWCO_{ti} - 0.087 \cdot P_{ti}, \qquad \forall t \in NF,\, i \in I_t,\, c \in COD \quad (2.14)$$

$$R_{tic} = 1.029 - 0.00037 \cdot MWCO_{ti} + 0.001 \cdot P_{ti}, \qquad \forall t \in NF,\, i \in I_t,\, c \in DOC \quad (2.15)$$

RO rejection coefficient for salt is presented in Eq.(2.16) as a function of the operating pressure [Chen and Guanghua, 2005].

$$R_{tic} = 0.890 + 0.340 \cdot P_{ti} - 0.003 \cdot P_{ti}^2, \qquad \forall t \in RO1,\, i \in I_t,\, c \in TDS \quad (2.16)$$

The above equation was derived following a study on ROSA software developed by The Dow Chemical Company [2013]. The TDS of interest were composed of K, Na, Mg, Ca, Ba, Sr, CO_3, HCO_3, NO_3, Cl, F, SO_4 and NH_4.

Boron (B) removal is identified as one of the main issues in processes where saline water is treated, especially because its concentration in seawater, in particular, is relatively low [Li et al., 2008]. Typical water treatment plants with source water containing boron, accommodate an RO pass at an elevated pH, where mainly removal of boron is targeted [Tu et al., 2010]. Therefore, its rejection profile is to be considered separately, with an RO unit dedicated to its removal. The regression equation (Eq.(2.17)) for rejection of boron by a RE4040-SH - module spiral wound RO membrane was derived based on data from literature [Mane et al., 2009], using ANOVA analysis.

$$R_{tic} = 0.408 + 0.046 \cdot pH_{ti} + 0.03 \cdot P_{ti}, \qquad \forall t \in RO2,\, i \in I_t,\, c \in B \quad (2.17)$$

where pH_{ti} is the alkalinity of the solution to achieve desired separation.

2.3.1.2 Recovery ratio

For any process, it is essential to meet the production quantities which depend on the productivity, or recovery, of the system. The recovery ratio is defined as the fraction of product water that has passed through the process unit from the overall feed. As a fraction, it takes values between 0 and 1. Over a technology and pass, it can be expressed by Eq.(2.18).

$$Y_{ti} = \frac{Q^P_{ti}}{Q^F_{ti}}, \qquad \forall t,\, i \in I_t \tag{2.18}$$

where Q^P_{ti} and Q^F_{ti} are the permeate and feed flowrates, respectively, associated with a technology t and pass i.

The recovery is a function of the salinity of the feed water, system pressure and scaling potential [Li et al., 2008]. However, in this work the recoveries for every different technology are assumed to take values recommended in literature and therefore, are modelled as parameters.

2.3.2 Mass balance constraints

2.3.2.1 Concentrations constraints

The set of equations below determines the contaminants concentration profile throughout the separation process. When a technology, t, and a pass, i, are selected, the binary variable, $\mathrm{W_{ti}} = 1$, and the contaminant is reduced, starting from an initial feed concentration, $\mathrm{c^{IN}_c}$. Eq.(2.19) estimates the contaminant concentration after the first selected process pass, i.e. the concentration in the permeate. Every consequent concentration reduction is calculated by Eq.(2.20). Eq.(2.21) and Eq.(2.22) show the interconnection between two potential candidate passes and technologies.

$$c^P_{tic} = c^{IN}_c \cdot (1 - R_{tic}) \cdot W_{ti} + c^{IN}_c \cdot (1 - W_{ti}), \qquad \forall t \in CF, i = 1, c \in C_t \tag{2.19}$$

$$c^P_{tic} = c^F_{tic} \cdot (1 - R_{tic}) \cdot W_{ti} + c^F_{tic} \cdot (1 - W_{ti}), \qquad \forall t, i \in \hat{I}_t, c \in C_t \tag{2.20}$$

$$c^P_{t,i-1,c} = c^F_{tic}, \qquad \forall t, i \in I_t, i > 1, c \in C_t \tag{2.21}$$

$$c^P_{t-1,i,c} = c^F_{tjc}, \qquad \forall t > 1, i = I^{max}_t, j = 1, c \in C_t \tag{2.22}$$

A similar formulation is implemented in previous works in applications for chromatography processes [Vasquez-Alvarez and Pinto, 2004, Polykarpou et al., 2012].

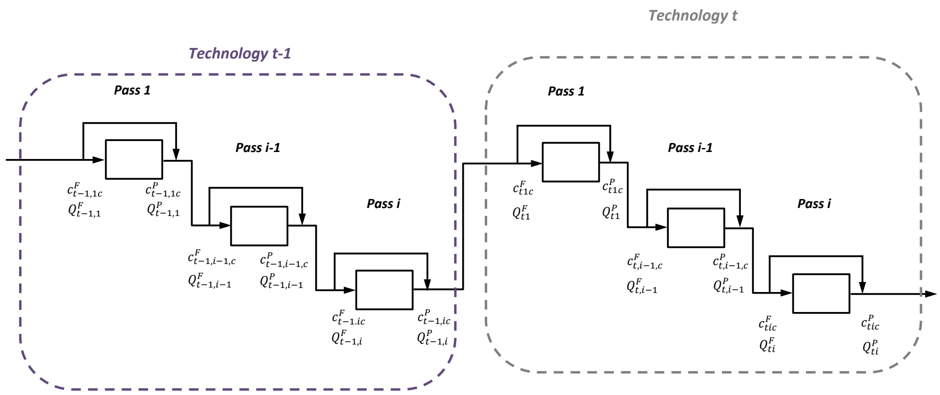


FIGURE 2.5: Schematic representation of two potential candidates

A schematic representation of the connections between two candidates is depicted in Fig. 2.5.

2.3.2.2 Flowrate constraints

Similarly, the flowrate constraints are formulated. When a candidate is selected, the permeate is calculated using Eq.(2.18). Otherwise it takes the value of the feed. Eq.(2.23) gives the initial mass balances starting from initial flowrate, Q^{IN}, and every consequent permeate is estimated from Eq.(2.24).

$$Q^P_{ti} = Q^{IN} \cdot Y_{ti} \cdot W_{ti} + Q^{IN} \cdot (1 - W_{ti}), \qquad \forall t \in CF,\ i = 1 \tag{2.23}$$

$$Q^P_{ti} = Q^F_{ti} \cdot Y_{ti} \cdot W_{ti} + Q^F_{ti} \cdot (1 - W_{ti}), \qquad \forall t, i \in \hat{I}_t \tag{2.24}$$

where Y_{ti} is the recovery of a technology t from pass i. The clarification technology takes either the recovery value of sedimentation or the recovery value of dissolved air flotation, shown in Eq.(2.25).

$$Q^P_{ti} = Q^F_{ti} \cdot (\sum_{s \in TCLR} \bar{Y}_{si} \cdot X_{si}) + Q^F_{ti} \cdot (1 - \sum_{s \in TCLR} X_{si}), \qquad \forall t \in CLR,\ i \in \bar{I}_s \tag{2.25}$$

The principles of designing the interconnections, whether a technology is selected or not, are formulated below.

$$Q^P_{t,i-1} = Q^F_{ti}, \qquad \forall t, i \in I_t, i > 1 \tag{2.26}$$

$$Q^P_{t-1,i} = Q^F_{tj}, \qquad \forall t > 1, i = I^{max}_t, j = 1 \tag{2.27}$$

The effluent is governed by the number of passes for a particular technology. The feed and permeate flowrates are modelled to present single-stage, multiple-pass system over each pass.

The annual production rate of the facility is then modelled by Eq.(2.28).

$$Q^{AP} = t_h \cdot t_d \cdot PY \cdot Q^P_{ti}, \qquad \forall t = T, i = I^{max}_t \tag{2.28}$$

where t_h and t_d are the respective operating hours per day and days per year. PY is the production yield of the facility, taking the value of a fraction of the total annual production capacity.

2.3.3 Target constraints

The final water purity should satisfy the conditions imposed by the following constraint:

$$c^P_{tic} \leq M^{CONC}_c, \qquad \forall t \in RO2, i = I^{max}_t,\ c \tag{2.29}$$

where M^{CONC}_c is the maximum allowable concentration of a contaminant. Depending on the process application, the final required concentration can take different values. An additional constraint for the minimum effluent at the final stage is enforced by Eq.(2.30).

$$Q^P_{ti} \geq M^{FLOW}, \qquad \forall t \in RO2,\ i = I^{max}_t \tag{2.30}$$

where M^{FLOW} is the minimum allowable effluent flow. This constraint allows us to ensure a minimum plant capacity is met.

2.3.4 Logical constraints

The overall number of the selected passes and technologies should not be greater than a number, N_{max}, which is modelled by Eq.(2.31).

$$\sum_t \sum_{i \in I_t} W_{ti} \leq N_{max} \tag{2.31}$$

Eq.(2.32) is a logical condition that does not allow the selection of any pass if the previous one has not been chosen.

$$W_{t,i+1} \leq W_{t,i}, \qquad \forall t, i \in I_t, i+1 \in I_t \tag{2.32}$$

The clarification processes, sedimentation and dissolved air flotation, have to be chosen together with the chemical treatment, coagulation-flocculation. Hence, the Eq.(2.33) applies:

$$\sum_{i \in \bar{I}_s} X_{si} \leq U \cdot \sum_{i \in I_t} W_{ti}, \qquad \forall s \in TCLR, t \in CF \tag{2.33}$$

where U is a big number that takes the maximum number of allowed passes per technology. Only one of the clarification processes can be chosen at a time, a condition expressed by Eq.(2.34).

$$\sum_{s \in TCLR} X_{si} = W_{ti}, \qquad \forall t \in CLR, i \in I_t \tag{2.34}$$

The same condition as in Eq.(2.32) is introduced for the clarification technologies.

$$X_{s,i+1} \leq X_{s,i}, \qquad \forall t, i \in \bar{I}_s, i+1 \in \bar{I}_s \tag{2.35}$$

2.3.5 Cost constraints

Defining water treatment costs at a preliminary stage often proves intricate due to the numerous factors participating in their estimation. Such factors are plant size, source and quality of feed water, site location and accessibility to electricity, distance from final users, qualified labour, energy costs and estimated plant life [Zhou and Tol, 2004]. All of them come under the operating or capital costs of treatment facilities, as the majority of them are included in the cost estimates demonstrated in the subsequent subsections.

2.3.5.1 Operating costs

The operating costs in coagulation are primarily accounted for by chemical consumption. They are determined by the dosage and the price per metric tonne of product. In the case of desalination, ferric chloride is often predominating due to the more satisfactory results obtained downstream. Aluminium sulphate (alum) and ferric sulphate have exhibited more solid outcomes in water and wastewater applications, hence, the preferred types of coagulant. The annual cost for the chemical is calculated from Eq.(2.36).

$$CHC = \sum_{i \in I_t} cv^{CHC} \cdot CD_{ti} \cdot C_{chem} \cdot t_h \cdot t_d \cdot (Q^{IN}|_{i=1} + Q^F_{ti}|_{i>1}) \cdot W_{ti}, \qquad \forall t \in CF \quad (2.36)$$

where $cv^{CHC} = 10^{-6}$ is a conversion factor, t_d is the number of operating days a year, t_h is the number of operating hours a day, CD_{ti} is the coagulant dose selected and C_{chem} is the cost of coagulant that alters in accordance with the type of coagulant. The dosage level mostly lies between the range of 0.5 to 100 mg/L of water as specifically it is between 10 to 30 mg/L for alum [Cheremisinoff, 2002, Energie- en Milieu-Informatiesysteem, 2010].

The electricity cost for the slow mixing in the flocculant tank, is given by Eq.(2.37).

$$EMC = \sum_{i \in I_t} cv^{EM} \cdot C^E \cdot t_d \cdot t_h \cdot \mu \cdot tf_{ti} \cdot (Q^{IN}|_{i=1} + Q^F_{ti|i>1}) \cdot Gf^2_{ti} \cdot W_{ti}, \qquad \forall t \in CF \quad (2.37)$$

where $cv^{EM} = 16.67 \cdot 10^{-6}$ is conversion factor for the electrical mixing equation. In Eq.(2.37), μ is the dynamic viscosity of the fluid and C^E is the electricity charge, and the power required is calculated for an accumulative number of chambers.

The technical and economic performance of DAF depends mainly on its recirculation ratio and saturator. The former is disregarded in this study and operating cost of the saturator, SC, is calculated by:

$$SC = \sum_{i \in I_t} \frac{cv^{SC} \cdot C^E \cdot Q^F_{ti} \cdot \bar{P}_{si} \cdot X_{si}}{\eta^{SAT}}, \qquad \forall t \in CLR, s \in DAF \quad (2.38)$$

where $cv^{SC} = 3.6^{-1}$ is the conversion factor for the equation, η^{SAT}_t is the efficiency of the saturator, $\bar{P}_{ti}$ is the saturator pressure, assumed to be the pressure supplied by the pump and C^E is the electricity cost rate.

The greatest contribution to the operating costs is derived from electricity, and more specifically, electricity for flowrates distribution and achieving separation pressure. Hence, the feed pumps are the main electricity consumers and their costs, denoted as PC, are expressed in the following equation.

$$PC = \sum_{t} \sum_{i \in I_t} \frac{cv^{PC} \cdot C^E \cdot (Q^{IN}|_{i=1} + Q^F_{ti}|_{i \in M}) \cdot P_{ti} \cdot W_{ti}}{\eta_t^{FP} \cdot \eta_t^{MT}} \tag{2.39}$$

$cv^{PC} = 3.6^{-1}$ is a conversion factor for the pumping cost equation. No pumps are assigned to the clarification processes in order to avoid breaking the flocs formed in CF.

The maintenance MCC and replacement MRC costs are also estimated by the number of passes.

$$MCC = \sum_{t \in TMM} \sum_{i \in I_t} af^{MCC} \cdot MC^O \cdot (D^{FM} + N^{MM} \cdot D^{VM}) \cdot W_{ti} \tag{2.40}$$

where af^{MCC} is an annualisation factor accounting for 2 times of major cleaning and maintenance in a year, MC^O is the operating cost charge rate during maintenance, N^{MM} is the number of modules in a unit and D^{FM} is fixed cost for downtime and D^{VM} is a variable cost during maintenance.

$$MRC = \sum_{t \in TMM} \sum_{i \in I_t} af^{MRC} \cdot MC^O \cdot N^{MM} \cdot RC^M \cdot W_{ti} \tag{2.41}$$

where af^{MRC} is an annualisation factor allowing membrane life of 5 years, i.e. $af^{MRC} = 0.2$ and RC^M is the membrane replacing cost per module.

The labour cost, LC, is the second largest expense in a manufacturing facility. Operators working hours requirements can be determined by examining the equipment flowsheet. The method for obtaining the labour cost is first, define the number of operators per shift for a given production rate, which is normally expressed in terms of a function of the number of separation units, as shown in Eq.(2.42) (Perry and Green [2007], KLM Technology Group [2014]).

$$LC = r^P \cdot t_d \cdot t_s \cdot n_s \cdot \sqrt{lc1 + lc2 \cdot \left(\sum_{t} \sum_{i \in I_t} W_{ti} \right)^2} \tag{2.42}$$

where r^P is the pay rate per person, t_s is the number of hours per shift, $lc1 = 6.29$ and $lc2 = 31.7$ are constants associated with the number of operators for all the units. The parameter n_s stands for the number of shifts per day.

For more than four decades, the EPA has used its authority to set cost-effective emission standards that ensure newly constructed sources use the best performing technologies to limit emissions of harmful air pollutants [Agency, 2014]. Owners or operators of facilities where aggregate annual green house gas (GHG) emissions are equal to or more than 25,000 metric tonnes of CO_2e must report to EPA under the Clean Air Act. Presently, EPA is not planning on requiring permits for sources that emit less than a 50,000 metric ton threshold until sometime after April 30, 2016 [McGuckin et al., 2013]. According to the same literature sources, although there is a continuous encouragement towards less emissions, there is no existing limit or taxes if limits are exceeded. With the view that policies of emissions tax will soon come to practice, the plant design can account for carbon taxes. They are calculated from Eq.(2.44) where the largest component for the emissions is the power used, reflected in the equation.

$$EMS_{ti} = cv^{Ems} \cdot CO_{2_e} \cdot t_d \cdot t_h \cdot P_{ti} \cdot (Q^{IN}_{i=1} + Q^{F}_{ti}|_{i \in \hat{I}_t}) \cdot W_{ti}, \qquad \forall t, i \in I_t \tag{2.43}$$

$$EMSC = \sum_t \sum_{i \in I_t} r^{CO_2} \cdot EMS_{ti} \tag{2.44}$$

where $cv^{Ems} = 3.6^{-1}$ accounts for the conversion factor for the carbon emission equation, CO_{2_e} is the carbon dioxide equivalent and r^{CO_2} is the carbon dioxide tax rate. Compared to pumping, the mixing footprint is relatively negligible, hence, not considered in the above constraints.

2.3.5.2 Capital costs

Capital costs for every plant are comprised of four major components, namely, project development, plant equipment and buildings, power supply, and piping and pumps [Blaikie et al., 2013]. In membrane plants especially, the equipment will include membrane elements, pressure vessels and passes. Despite the availability of tools for estimating capital cost, the assumptions in deriving those tools have not been clearly stated. When capital costs are estimated, inflation and other market factors should be taken into account in order to update existing cost models [Sethi, 1997]. Adham et al. [2006], sponsored by the U.S. Environmental Protection Agency (EPA) and AWWA Research Foundation, published correlations for the total construction costs of coagulation – flocculation. The European Commission issued a report on best available techniques in water treatment with construction costs for sedimentation [European Commission, 2003]. L.K. Wang and Aulenbach [2010] reported DAF construction costs for a specified volume. EPA published investment cost equations for production flow ranges [Whitman et al., 2002]. The cost estimation for low-pressure membranes plants, such as MF and UF, was expressed as the cost per unit produced water [of New Hampshire, 2016]. In an industrial study for high pressure membranes, a breakdown for the various capital cost components has been shown for different capacities [American Water Works Association Research Foundation et al., 1996]. All the equations can be combined under the common form below.

$$CC_{ti} = infl_t \cdot A_t \cdot (Q^P_{ti})^{b_t} \cdot W_{ti}, \qquad \forall t, i \in I_t \tag{2.45}$$

where $infl_t$ is inflation factor depending on the year of estimation, A_t and b_t are specific parameters for every technology. In all the cases, the parameter A_t was estimated from the reference capital cost and equipment capacities stated in literature. The capital cost for the clarification technologies is calculated from the expression below.

$$CC_{ti} = \sum_{s \in TCLR} infl_s \cdot A_s \cdot (Q^P_{ti})^{b_s} \cdot X_{si}, \qquad \forall t \in CLR, i \in I_t \tag{2.46}$$

The capital cost summed and multiplied by the capital recovery factor (CRF) to obtain the total annual capital cost, ACC, is given in Eq.(2.47).

$$ACC = CRF \cdot \sum_{t} \sum_{i \in I_t} CC_{ti} \tag{2.47}$$

as the CRF is expressed in Eq.(2.48).

$$CRF = \frac{ir}{1 - \frac{1}{(1+ir)^{yr}}} \tag{2.48}$$

where ir is the bank interest rate and yr is the number of years for investment which often coincides with the plant life.

2.3.5.3 Total cost

The total annual cost, TC, is a sum of the chemical CHC, mixing EM, saturator SC and pumps PC running costs, membrane cleaning costs MCC, membrane replacement costs MRC, labour cost LC, emissions cost $EmsC$ and the annual capital costs ACC

for all the selected technologies.

$$TC = CHC + EMC + SC + PC + MCC + MRC + LC + EMSC + ACC \quad (2.49)$$

2.3.6 Objective function

The objective function is to minimise the water net cost, WNC, which is equal to the total annual cost divided by the annual plant production rate:

$$minimise \quad WNC = \frac{TC}{Q^{AP}} \quad (2.50)$$

which is subject to:

- separation efficiency Eqs.(2.5) - (2.17)
- mass flow balance Eqs. (2.19) - (2.28)
- target purity Eq. (2.29) and final effluent Eq. (2.30)
- logical conditions Eqs.(2.31) - (2.35)
- operating costs Eqs.(2.36) - (2.44)
- capital costs Eqs.(2.45) - (2.47)
- total annual cost Eq.(2.49)

Along with minimising the major capital investment and the annualised operating cost with the objective function, it is aimed to minimise the number of passes for achieving maximum final water purity, and increase the capacity of the facility. The applicability of the proposed method is manifested through two case studies discussed in the next section.

2.4 Illustrative examples

2.4.1 Seawater desalination example

Abundance grants seawater the opportunity to be a major solution to water scarcity. Thus, the first case study in the present work focuses on seawater desalination for the production of potable water. For the case study the influent, $Q^{IN} = 55,000\, m^3/h$, as to agree with existing practices. The minimum allowable effluent $M^{FLOW} = 5,000\, m^3/h$, resulting in a minimum $120,000\, m^3/d$, i.e. medium - to - large size facility [Cipollina et al., 2009]. For the influent and effluent, it is essential to determine the initial contaminants concentration in seawater and the final requirements for drinking water. The American Water Works Association [American Water Works Association, 2007] reported typical seawater intake qualities in the range $30,000 - 40,000\, mg/L$ TDS.

TABLE 2.1: Feed water characteristics and final purity requirements

Contaminant s	Initial concentration $c_c^{IN} [mg/L]$	Final concentration $M_c^{CONC} [mg/L]$
TDS	40 000	600
TSS	30	1
Boron	5	2.4

Source: Tchobanoglous et al. [2003], Mane et al. [2009], American Water Works Association [2007]

The selection of the technologies is based on meeting the health regulatory requirements for potable water [The Drinking Water Inspectorate, 2009, U.S. Environmental Protection Agency, 2010]. The World Health Organization [2011] reported drinking water of good quality contains less than ca. 600 mg/L TDS. Although, no explicit limits exist in the Drinking Water Quality Guideline regarding TSS, they can be correlated to turbidity, which should not exceed 1 NTU, and in many cases 0.5 NTU [Gallegos, 1993]. Thus, the final purity specification used in the model is less than 1 mg/L TSS. The World Health Organization [2011] revised the maximum allowable concentration of boron in drinking water from 0.5 mg/L in 2003 to 2.4 mg/L and the latter value is the final purity requirement in the model. The initial and final water characteristics are listed in Table 2.1.

TABLE 2.2: Operating conditions boundaries

Operating conditions	Range
$\mathrm{CD_{ti}}$ $[mg/L]$	1 - 20
$\mathrm{Gf_{ti}}$ $[s^{-1}]$	10 - 120
$\mathrm{tf_{ti}}$ $[min]$	5 - 35
$\mathrm{D_{ti}}$ $[mm]$	2.0 - 8.0
$\mathrm{Ld_{ti}}$ $[m/h]$	0.5 - 1.5
$\mathrm{L_{ti}}$ $[m]$	0.5 - 2.5
$\mathrm{Temp_{ti}}$ [°C]	20 - 30
$\mathrm{H_{ti}}$ [-]	-6.2 - 0.0
$\mathrm{MWCO_{ti}}$ [Da]	300 - 1200
$\mathrm{pH_{ti}}$ [-]	7.5 - 9.5

Source: Cheremisinoff [2002], Vlaški [1998], Lin et al. [2006], Lu et al. [2006], Bastaki [2004], Hassan et al. [1999]

The operating condition boundaries are determined next. Literature suggests recoveries for MF and UF systems between 85% and 95% which reach 100% depending on the flow configuration [US Interior Reclamation Department, 2013]. In the current case study, the recoveries of the low pressure membranes are modelled with the assumption of a full flow recovery. Typical system recoveries for NF membranes take values between 75% and 90% whereas they vary from 35% to 50% for RO systems [Lu et al., 2006, Mickley et al., 2006]. Based on reported values, recoveries of 80% for NF and 40% for RO are adopted in the model.

In his experimental work, Vlaški [1998] varied the energy input to the flocculation tank from 10 to 120 s^{-1} and flocculation time from 5 to 35 min to investigate the performance of downstream clarification processes. The chosen boundaries coincide with the values used in the experiments. CSIRO performed experiments where the grade of media were 2.18, 5.18 and 7.55 mm in diametre, the load values attempted were 0.5, 1.0 and 1.5 m/h, and the filters lengths were 0.6, 1.2, 1.8, 2.4 m [Lin et al., 2006]. The values taken in the case study are rounded down to 2 mm for lower bound and 8 mm for upper bound for diametre. The rest of the boundaries are presented in Table 2.2.

It is assumed that cleaning or replacement takes place simultaneously for all passes, there are no pressure losses from pump to membrane, every pass contains the same number of membrane modules, $N^{MM} = 360$, cleaning is performed every 6 months, replacement is recommended every 5 years, and the annual operation is 300 days a year. The electricity charge, C^E, has a value of 0.08 $US\$/kWh$ to accommodate any future increments from the U.S. Energy Information Administration [2013] review and to consider literature values [Lu et al., 2006].

Table 2.3: Operating costs parameters data

Parameter	Value
Number of modules, $N^{MM}[-]$	360
Electricity cost, C^E[US$/kWh]	0.08
Operating cost charge during maintenance, MC^O[US$]	0.2
Membrane replacing cost per module, RC^M[US$]	800
Fixed cost for downtime during maintenance, DC^{CM}[US$]	200
Ferric coagulant cost, C_{chem}[US$/tonne]	250
Carbon dioxide equivalent, CO_{2_e}[kg/kWh]	1.31
Carbon dioxide rate, r^{CO_2}[US$/kg]	0.023
Seawater viscosity, μ[kg/m $\cdot$ s^2]	$1.307 \cdot 10^{-3}$
Operating hours a day, $t_h[h/d]$	24
Operating days a year, $t_d[d/y]$	300

Source: UNESCO Centre for Membrane Science and Technology [2008], National Physical Laboratory [2015], Lu et al. [2006]

Table 2.4: Pressure design variables, and efficiency and economic parameters

Technology	CF	CLR SED / DAF	MMF	MF	UF	NF	RO1	RO2
P_{ti} [MPa]	0.1 - 0.2	- / 0.4 - 0.7	0.1 - 0.2	0.1 - 0.2	0.1 - 0.3	0.5 - 1.6	5.0 - 6.0	5.0 - 6.0
η_t^{FP}	0.75	- / 0.75	0.80	0.80	0.75	0.80	0.75	0.75
η_t^{MT}	0.95	- / 0.95	0.93	0.95	0.97	0.95	0.98	0.98
$infl_t$	1.143	1.288/1.087	1.319	1.087	1.087	1.511	1.511	1.511
A_t	121,701	8,334 / 4,167	69,547	45,601	45,601	158,177	158,177	158,177
b_t	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6

Source: Lu et al. [2006], Bastaki [2004], Hassan et al. [1999], US Inflation Calculator [2013]

To consider updating of the capital costs, the plant location has to be determined. Assuming the facility to be built in the U.S., the inflation for the capital costs from the reference year of citation has been considered. The consumer price indices (CPI) for those years, together with the inflation rates, are reported in Table 3.4, where the CPI for year 2014 was 236.7 [US Inflation Calculator, 2013]. The term of bank loan was taken as yr = 30 years, the interest rate was assumed to be ir = 6% and the plant was considered to produce 95% of its design annual yield based on standard practices [American Water Works Association, 2011]. The rest of the design parameters are given in Table 2.3 and Table 3.4. Whenever values in literature could not be found, assumptions and approximations were used in accordance with practical cases. Finally, the carbon emissions have been calculated assuming no carbon taxation.

2.4.2 Tertiary wastewater treatment example

Water reclamation and advanced water treatment have recently faced significant enhancement due to membrane improvement. Thus, the second case study focuses on tertiary wastewater treatment for the production of potable water.

It is assumed that wastewater, with the characteristics listed in Table 2.5, enters the purification system.

Table 2.5: Feed water characteristics and final purity requirements

Contaminant s	Initial concentration $c_c^{IN}[mg/L]$	Final concentration $M_c^{CONC}[mg/L]$
COD	70	5
DOC	8	2
TDS	15,000	600
TSS	200	1
Boron	2.4	2.4

Source: Tchobanoglous et al. [2003], Cheremisinoff [2002], Chowdhury et al. [2013]

The main characteristics of wastewater impose taking into account the organic matter, such as COD and DOC, in the case study. The initial secondary effluent concentrations were decided based on similar values in literature [K.Wang and Zhao, 2014, Nieuwenhuijzen and Graaf, 2011, C. Kaznaer and Dillon, 2012]. No standards have been mentioned for the maximum contaminant level (MCL) by the World Health Organisation. However, a number of sources declare ≤ 5mg/L for COD and roughly ≤ 2 mg/L for DOC drinking water quality at neutral pH [C. Kaznaer and Dillon, 2012, P. Fox and Reinhard, 2001].

Boron is an issue specifically for seawaters, therefore, in this case study, it was assumed its influent concentration equals to the required concentration of boron in drinking water. As the total dissolved solids concentration is significantly lower, the reverse osmosis systems will work with higher recoveries. For the case study, a value of 0.6 was assumed.

According to the application, aluminium sulphate (alum) coagulant/flocculant is used. Its dosage is reported to be in the standard range of 10 to 30 mg/L for treatment of suspended solids [Cheremisinoff, 2002]. Organics necessitate a higher dose, hence, up to 50 mg/L dose was allowed as performed in experiments [K.J.Howe and Clark, 2002]. The price of alum can be found at approximately $US\$\,150/tonne$ [Global B2B Marketplace, 2015]. Additionally, viscosity value of $1.002\,kg/m \cdot s$ at ambient temperature was taken.

The rest of the data overlaps with the given data from Section 2.4.1.

2.5 Computational results and discussion

2.5.1 Seawater desalination results

The model was solved in GAMS 24.4 [Rosenthal, 2012] on a Dell PC OptiPlex 9010, Intel Core i7 - 3770 CPU at 3.4 GHz and 16 GB RAM. Its computational statistics involve 40 binary variables, 564 continuous variables and 569 constraints. The model was solved by ANTIGONE which returned a solution within 48.8 seconds, with an optimal gap 0. The branch - and - bound solving technique was satisfactory for achieving the optimal solution.

Flowsheet configuration

The optimal sequence of process units comprised three ultrafiltration passes, primarily from fouling. Altogether they served as a pretreatment system to the desalting section. Two nanofiltration and one reverse osmosis passes were chosen, the former for the TDS removal and the second one for the boron removal (Fig. 2.6).

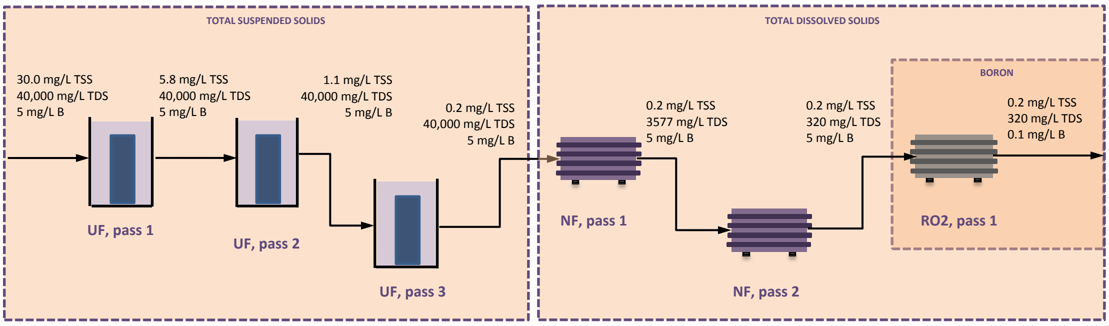


FIGURE 2.6: Optimal flowsheet configuration for the desalination case study

Operating conditions

Table 2.6 summarises the operating conditions returned by ANTIGONE. The predominant results lie in the lower bounds of the variables, showing the constraints are active. On the other hand, lower power translates into lower costs. It is also worth mentioning that some of the technological characteristics, such as molecular weight cut - off, hydrophobicity and pH, do not influence the operating costs directly. This might result in observing differences in the final purities, when there is a nanofiltration and reverse osmosis selected, while the water net cost will remain the same with various non-linear solvers or few runs with one solver. The reason for this observation lies in the exclusion of chemicals costs for altering the alkalinity of the feed and also, in the assumption of no fouling occurring, where cleaning cycles and replacement can be predicted by the pore size of the membranes.

Cost

The largest contributor to the operating costs was the electricity, followed by the labour cost, representing 21% of the operating costs. The cleaning and replacement costs were

Table 2.6: Operating conditions for seawater case study

Operating condition	Range
P_{UF} [MPa]	0.1
P_{UF} [MPa]	0.1
P_{NF} [MPa]	0.5
P_{RO2}[MPa]	5.0
Tem_{MF} [°C]	20
$MWCO_{NF}$ [Da]	300
H_{NF} [−]	0.002
pH_{RO2} [−]	8.0

relatively insignificant due to the fixation of the number of membrane modules, no cleaning chemicals costing and assumption of activities repetitiveness.

In 2012 IWA published a book dedicating a chapter on seawater desalination where the water net cost lay between $US\$\,0.5/m^3$ and $US\$\,3.0/m^3$, depending on the capacity of the facility [Lazarova et al., 2012]. The optimal solution returned by ANTIGONE was $US\$\,1.044/m^3$ with a daily production of $337,920\,m^3/d$ and consequently, the result fell into the suggested limits. In addition the report by UNESCO from 2008 gives unit costs of the desalination plants in Perth ($150,000\,m^3/d$) and Sydney ($250,000\,m^3/d$) with total product costs $US\$\,1.16/m^3$ and $US\$\,2.29/m^3$, respectively. It should be noted that the transportation costs for a distance of 100km for those plants is less than $US\$\,0.06\,/m^3$, meaning the water net cost will not be significantly influenced if they are added to it.

Sensitivity analysis

Next, sensitivity analysis was performed for the number of passes per technology, maximum number of passes, influent contaminants fluctuation, and interest rates and plant life.

Sensitivity analysis of passes

In the case study four number of passes for every technology were allowed. It was then investigated how the results change with the number of passes. It is expected that global solvers do not experience any changes down to two passes as this is the maximum number from a technology returned in the optimum solution. For $i = 1$, however, ANTIGONE returned water net cost $UUS\$\,2.105/m^3$ with flowsheet configuration shown in Fig. 2.7.

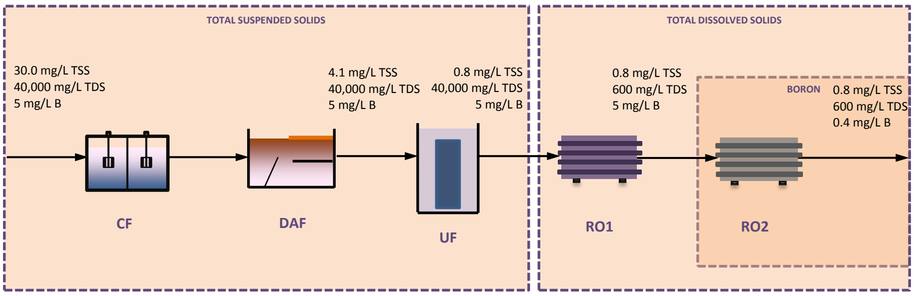


FIGURE 2.7: Optimal flowsheet configuration for the desalination case study with one pass

Next, the total allowable number of passes was decreased. In the case study, out of 10, the global solvers return 6 passes, meaning the solution would not change if $N_{max} > 6$. When $N_{max} = 5$, the water net cost returned was $US\$\,1.982/m^3$ with a configuration MF - 2xNF - RO1 - RO2 (Fig. 2.8).

Selecting more passes of the same technology leads to economically more favourable flowsheets. In the studied case, the difference in price is due to the coagulant cost for the CF unit and its capital. The flowsheet in Fig. 2.8 differs from the optimal solution, presented in the previous subsection, by the RO pass for TDS removal. Pumping cost is, thus, the major contributor to the difference in price between the two.

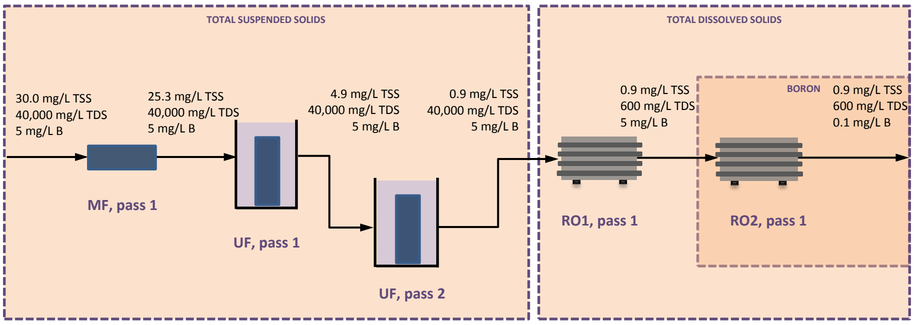


FIGURE 2.8: Optimal flowsheet configuration for the desalination case study with overall maximum number of passes 5

Sensitivity analysis of TDS and TSS

Seawater desalination plants are exposed to daily and seasonal contaminant variations. Hence, it is necessary to explore how the flowsheet can alter or what the fluctuation in final purity of the initially selected flowsheet will be. The TDS concentration was varied from $20,000\,mg/L$ to $40,000\,mg/L$ with a step change $5,000\,mg/L$. No changes occurred in the flowsheet configuration and water cost, meaning the system is overdesigned with respect to total dissolved solids and it is capable to handle feed variations and still meet model restriction criteria. Another reason is already the mentioned technological characteristics which do not affect the final cost, meaning fluctuations in TDS would not change the flowsheet significantly unless additional constraints are introduced or NF is no longer able to remove the contaminant group down to the required purity.

Although fluctuations in dissolved solids are likely, it is more likely that the seawater is exposed to turbidity variations due to weather conditions, recycled water streams that were directed to the sea, etc. Thus, the change of suspended solids feed concentrations was studied by varying it from $20\,mg/L$ to $40\,mg/L$. Not only did the final TSS concentration alter but also the choice of technologies in the relevant section and the final product cost (Fig. 2.9). The water cost increases with TSS because of the need for higher number of passes or more efficient technology. As Eqs.(2.8) and (2.10) suggest, for separation of higher TSS concentration, more units and with higher pressure will be selected. Therefore, the increase in price stems from the electricity cost for pumping. From an engineering perspective, the most robust flowsheet, out of the three options, is the configuration which can handle largest contaminant fluctuations, i.e. the third option.

Sensitivity analysis of carbon emissions

The designed facility would annually emit greenhouse gases at the rate $634,040\,tonnes/year$, 49% less than the desalination plant in Sydney, for instance, while exceeding its production by 33% [UNESCO Centre for Membrane Science and Technology, 2008]. Other sources have demonstrated that the range of kilogram emissions per volume of water produced can vary from $2.03\,kg/m^3$ in Spain to $7.80\,kg/m^3$ in Australia [Lattemann, 2010]. The emissions produced for the designed conceptual flowsheet do not exceed $6.25\,kg/m^3$. Current regulatory practices will impose official annual reporting to EPA. To reflect future intentions of environmental regulatory bodies, an option of carbon taxation of $US\$\,0.023/CO_2\,kg$ was studied in the model. The option affected the flowsheet configuration by substituting one of the pretreatment ultrafiltration passes with a microfiltration. Thus, the emissions and their respective taxation would decrease while the

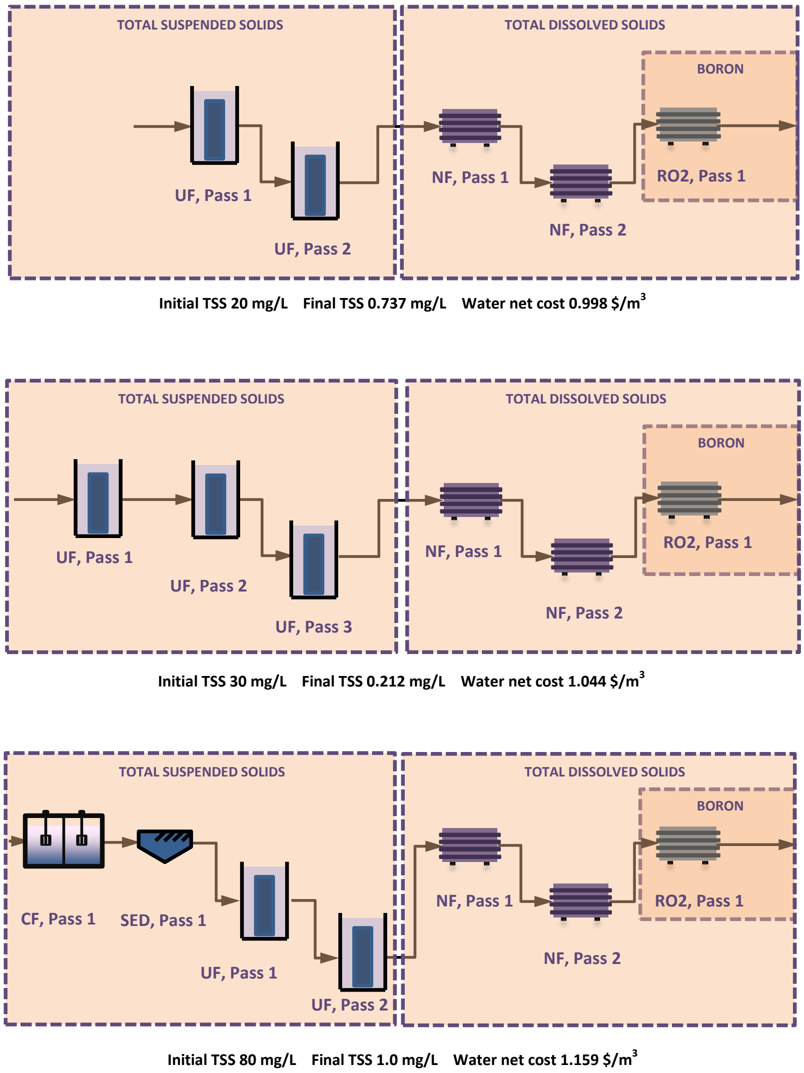


FIGURE 2.9: Flowsheet changes with TSS fluctuations

water quality would be still met. The water net cost rose to $US\$\,1.195/m^3$, approximately 14% difference in comparison to the WNS from the base case.

Sensitivity analysis of interest rate and plant life

Local authorities in the US provide financing through low-interest loans and such initiatives are a common practice for boosting water treatment facilities commissioning [US Environmental Protection Agency, 2015]. Hence, it is worth examining the water cost modifications at different interest rates and designing for shorter and longer plant lifetimes.

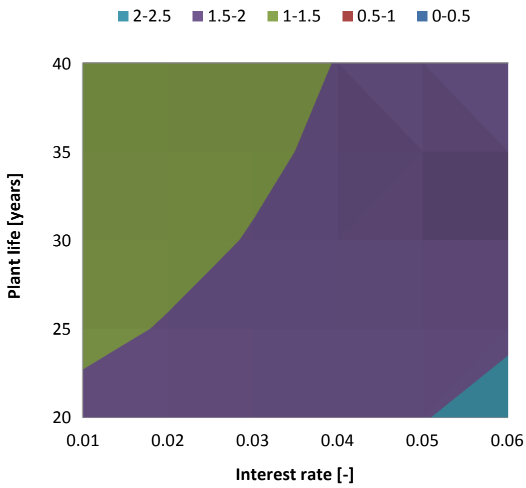


FIGURE 2.10: Water net cost change with bank interest rate and plant life time

From Fig. 2.10 it is observed that the lower cost range will lie in the low interest rate - short plant lifetime and high interest rate - longer plant lifetime area. The minimum water cost is $US\$ \, 0.846/\, m^3$ at 1% interest and 40 years project scope. Under these conditions the water net cost undergoes nearly 23 % reduction as a result of the decrease in annual capital cost. Currently, the design integrates one of the worst case scenarios where no governmental incentives are available. From this follows the higher unit cost.

2.5.2 Tertiary wastewater treatment results

For the second case study with 715 constraints and 730 continuous variables, it took ANTIGONE 204.18 seconds to return a solution, with an optimality gap 0.

Flowsheet configuration

The advanced wastewater treatment flowsheet consisted of one coagulation-flocculation process unit, followed by a sedimentation step. Two nanofiltration units were allocated for the removal of the organic matter and the total dissolved solids. This flowsheet configuration is common for water and advanced wastewater treatment. A schematic of the optimal flowsheet is given in Fig. 2.11.

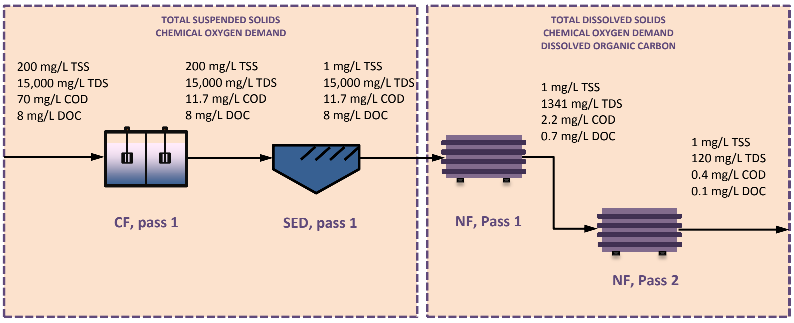


FIGURE 2.11: Optimal flowsheet configuration for the advanced wastewater treatment case study

Operating conditions

The operating conditions from the advanced wastewater treatment case study are reported in Table 2.7. Unlike in the previous case study, here, some of the operating conditions have inactive boundaries, such as coagulant dosage and hydrophobicity of the second NF pass. Consequently, the computational time increased.

TABLE 2.7: Operating conditions for advanced wastewater case study

Stage	ANTIGONE
CD_{CF} [mg/L]	30.7
pH_{CF} [−]	7.24
tf_{CF} [min]	5.0
Gf_{CF} [s^{-1}]	10.0
P_{NF} [MPa]	0.5

Cost

Al-Hamdi [2010] compared desalination and wastewater treatment where the unit costs reported only for advanced wastewater treatment are in the range $US\$\,0.31/m^3 - US\$\,0.6/m^3$. The values agree with other literature sources [Alhumoud et al., 2010, Tchobanoglous et al., 2003] that report values ca. $US\$\,0.5/m^3$ as the cost can drop down to around $US\$0.14/m^3$ [104] for large - scale plants. Compared to the aforementioned water net values, the obtained optimal solution lies in the low boundary of the given ranges, i.e. $US\$\,0.22/m^3$, for a designed facility with capacity of $802,560m^3/d$.

Advanced wastewater treatment for fit-for-purpose

Wastewater and advanced wastewater treatment in particular participate in projects for specific purposes other than drinking, e.g. industrial uses, agriculture, irrigation, etc. Such systems have lower water quality objectives in comparison with drinking water applications, and as a result, the level of treatment varies depending on the end use. Then, water quality for crops irrigation with the following quality was considered: TSS $30\,mg/L$, TDS $290\,mg/L$, B $0.75\,mg/L$ [National Research Council, 2012]. The flowsheet configuration was $2xUF/\,2xNF/\,RO2$ (Fig. 2.12) producing at water net cost $US\$\,1.236/\,m^3$ and the increase in cost is due to the necessity of boron treatment.

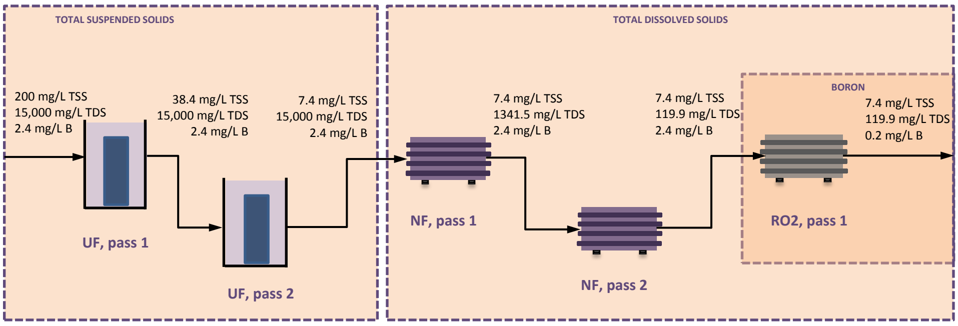


FIGURE 2.12: Optimal flowsheet configuration for the advanced wastewater treatment case study

Comparison between seawater and advanced wastewater case studies

Lastly, a comparison between the two case studies was conducted based on technologies selection and costs breakdown. Nowadays pretreatment systems can operate without sedimentation or dissolved air flotation. Sedimentation basins are capable of producing seawater with approximately less than $1\,mg/L$. This, however, depends on the source of water. If $TSS > 100\,mg/L$, SED is recommended to be installed [Voutchkov, 2010]. DAF is more energy intensive than SED and when the total suspended solids are high, the process is economically unfavourable. On the other hand, the processes are efficient for intense removal of TSS without the concerns about equipment fouling. With the assumption of no need for removing boron, the reverse osmosis becomes redundant. The choice of equipment pre-determines the operating costs of the systems. In Fig. 2.13 the breakdown costs per volume for both applications are presented. Seawater desalination

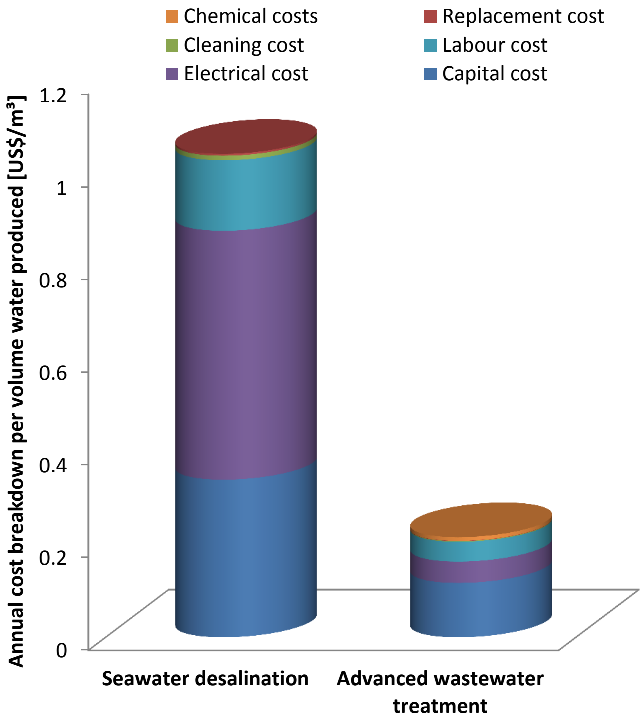


FIGURE 2.13: Annual cost breakdown comparison per volume of water

demonstrates approximately ten times higher electricity cost because of the pumping requirements in overcoming osmotic pressure of saline water. When the TSS is high, coagulants that treat the water are significantly less expensive while their dosage rise less than double at maximum. Therefore, CF becomes economically advantageous but accounts for the extra chemical cost. The labour cost per volume of water is significantly higher in seawater desalination due to the extra pass and lower production rate. The capital costs are relatively comparable as one of the flowsheets has four process units, and the other one - six. Future refinements of the mathematical model can lead to a more accurate representation of the physico-chemical system of water treatment.

2.6 Conclusions

In this work a systematic approach for the design and optimisation of water treatment processes has been proposed. The problem has been formulated as a mixed integer non-linear program model. The objective function minimises the water production cost manipulated by the techno-economic performance of the technologies selected. Two case studies have been presented with two applications, on seawater desalination and advanced wastewater treatment. The computational results have demonstrated an alignment with existing water engineering technical and economic practices which proved the applicability of the proposed approach and model.

Chapter 3

Synthesis of Water Treatment Processes with Passes and Stages

Chapter 3 advances the optimisation framework presented in Chapter 2 by introducing alternative paths in the superstructure. Simultaneously, it seeks to improve the computational performance of the resulting highly non-linear formulation by applying various linearisation and approximation techniques.

3.1 Theoretical background

Intricacy of water treatment design is, normally, due to bilinearities arising from mixing of streams of different qualities, which immensely increases the computational effort to achieve global optimality. Karuppiah and Grossmann [2006] and Castro [2015] have demonstrated the applicability of bilinear relaxations using McCormick envelopes in different problems, including wastewater treatment. Teles et al. [2012] implemented a multiparametric disaggregation technique for water networks design. Castro [2016] proposed a normalised multiparametric disaggregation (MDT) strategy which has been demonstrated to improve the convergence of non-convex problems. The technique has successfully been implemented in wastewater treatment applications [Ting et al., 2016].

This chapter presents a superstructure optimisation approach for the synthesis of water and water - related treatment processes by introducing essential new alternative paths to its superstructure in Chapter 2 and hence, illustrating more closely common industrial practices. Three mathematical formulations are developed, an MINLP model ($P0$), a partially linearised MINLP (plMINLP) model ($P1$) and a mixed integer linear fractional programming (MILFP) model ($P2$). The originality of the work lies in: (i) removal efficiencies modelled as continuous variables. Models $P0$ and $P1$ consider removal efficiencies as continuous variables whose values are determined by regression models with independent variables - the operating conditions of the treatment units; (ii) unique superstructure accommodating the technologies used across water, advanced wastewater treatment and desalination; (iii) operating costs breakdowns and capital costs for every candidate technology. The rest of the chapter is structured as follows: in Section 3.2 the superstructure optimisation problem is given together with the assumptions along its development and the problem statement. Next, the mathematical formulations are presented and the solution strategies are discussed in Section 3.3. The capabilities of the models are then tested on two case studies in Section 3.4 whose results are discussed and analysed in Section 3.5. Finally, Section 3.6 draws conclusions from the obtained results and summarises the major points from this work.

3.2 Problem statement

The aim of the current work is to develop a methodology for the generation of a combination of technologies that result in the most economically favourable flowsheet design. Similarly to Chapter 2, the proposed model accounts for contaminants classified into major groups such as total suspended solids (TSS), total dissolved solids (TDS), chemical oxygen demand (COD) and boron (B). Nine technology candidates are considered, i.e. coagulation-flocculation (CF), sedimentation (SED), dissolved air flotation (DAF), multi-stage media filtration (MMF), microfiltration (MF), ultrafiltration (UF), nanofiltration (NF), reverse osmosis (RO) for TDS (RO1) and B (RO2) removal. The acceptable connections among those technologies have been diversified and illustrated in the enhanced model superstructure in Fig. 3.1. Every technology is associated with the removal of a group or groups of contaminants.

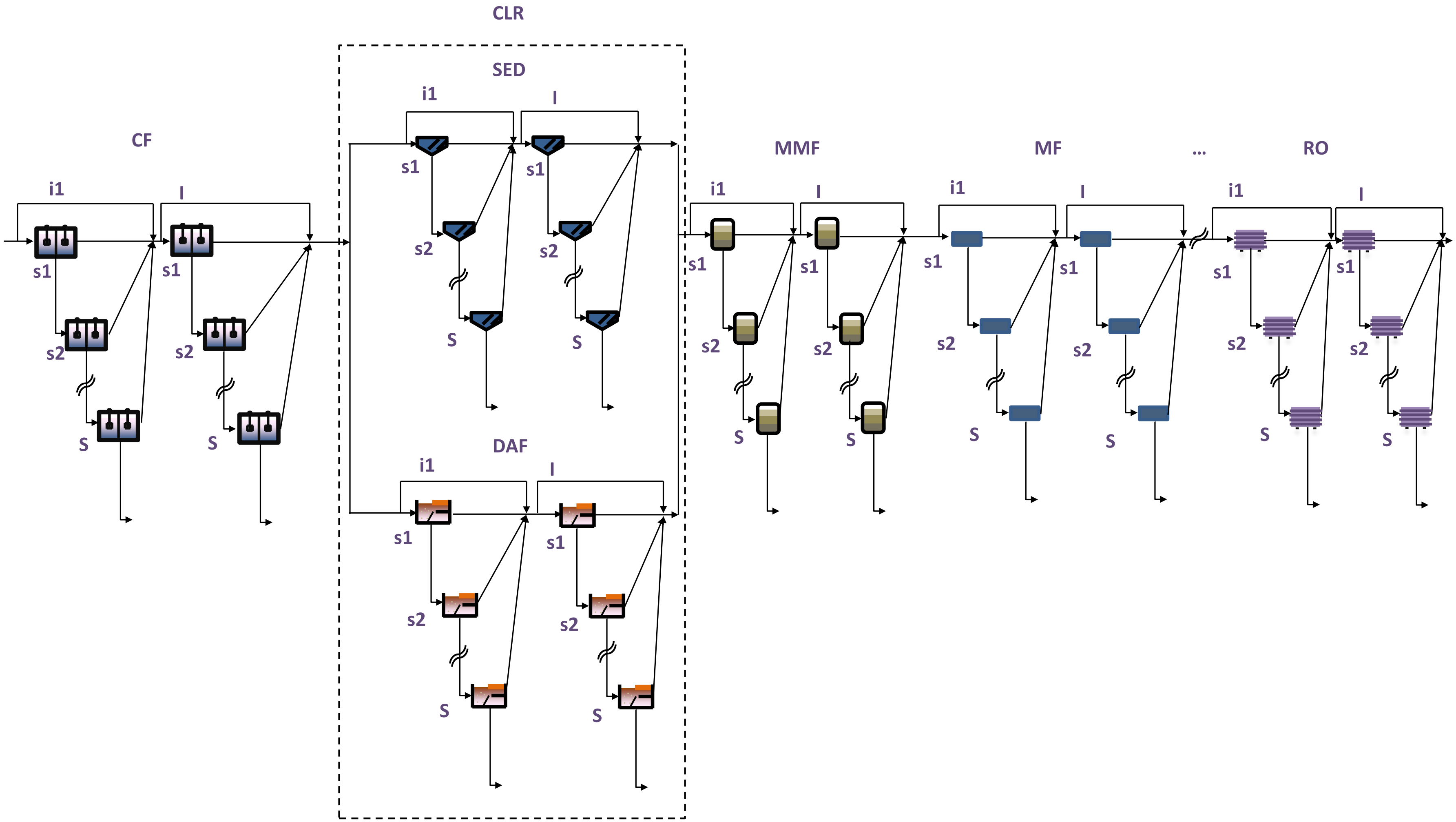


FIGURE 3.1: Process superstructure: coagulation-flocculation (CF), sedimentation (SED), dissolved air flotation (DAF), media filtration (MMF), microfiltration (MF), ultrafiltration (UF), nanofiltration (NF) and reverse osmosis (RO)

The sequence of the technology candidates in the model is pre-fixed in an order they are most commonly configured in established practices. A candidate, however, can be either selected or bypassed. In conventional treatment, coagulation-flocculation is followed by a clarification process. Two clarification options are provided, SED and DAF. They are represented by the collective name CLR which is symbolically depicted with a dotted line in the superstructure. Provided SED or DAF is selected, CLR is selected, too. A selection of a clarification process serves as a prerequisite for the selection of CF. Coagulation-flocculation alone can be selected if the separation is efficient enough. Low pressure membranes (MF and UF) and high pressure membranes (NF and RO) are allowed to exist sequentially in the superstructure. Nevertheless, the problem can be restricted to the selection of either of a membrane from a group.

Every unit can be repeated in a sequential manner, or a *pass*, denoted also by i. A pass is used in order to increase product purity. Every unit can be repeated to treat the concentrate or retentate of a preceding unit. This structure is referred to as *stage* and is denoted by s. A stage is used in order to increase the productivity of the system. Whether a pass and a stage from a technology are singled out is decided by a binary variable. Additionally, a technology can have as many number of passes and stages as economically viable. The unit selection is based on meeting the regulatory requirements depending on the purpose of water usage [The Drinking Water Inspectorate, 2009, U.S. Environmental Protection Agency, 2010]. The flowsheet configuration has to be such as to minimise the water net cost, expressed in US\$/m^3. The following assumptions have been made along the mathematical formulation development:

Assumptions

- removal efficiencies are the major technological criterion
- coefficients of determination are satisfactorily high for providing a good fit for removal efficiencies
- the major contaminant groups depend on water source; the rest are untraceable
- insignificant removal of a group of contaminants from technologies assigned for removal of other groups
- initial removal grids, intake screens and post-treatment equipment are not considered
- no fouling and flux decrease
- no system pressure losses
- cost indices can be grouped for lower pressure membranes (MF and UF) and high pressure membranes (NF and RO)
- plant shut down for maintenance takes 65 days
- annual water production and operating expenses do not fluctuate throughout the commercial lifespan of the plant
- no government incentives, such as decreased interest rate or no interest rate, apply

The overall optimisation problem can be stated as follows.

Given:

- contaminant groups and concentrations in intake
- industrially available treatment technologies
- maximum number of passes and stages allowed for a technology
- intake flowrate
- recoveries, pump and motor efficiencies for every unit
- candidate technologies characteristics ranges ($P0$ and $P1$) or discrete values ($P2$)(e.g. flocculation time and energy input, coagulant concentrations, operating pressures, influent temperature, hydrophobicity, hydrogen ion concentrations, molecular weight cut - offs)

- cost indices (e.g. units upfront costs, chemicals and electricity charges, equipment replacement rates, labour associated constants, interest rate and plant life)

Determine:

- process flowsheet including multiple-pass and multiple-stage strategy
- optimal removal efficiencies and operating conditions for the selected units
- contaminants and flowrates profiles
- annual operating and capital costs

So as to:

minimise the water production cost which is defined as the total annualised cost divided by the annual production rate.

3.3 Mathematical formulation

3.3.1 MINLP model formulation (P0)

3.3.1.1 Removal efficiencies

Meeting product specifications is the most important goal of the model which is achieved through the separation performance of the technologies composing a flowsheet. The physicochemical properties of the fluid and the operating conditions of the available technologies (PP_{tisc}) impact their separation efficiency and generically, can be stated as follows:

$$R_{tisc} = f(PP_{tisc}) = 1 - \frac{C^P_{tisc}}{C^F_{tisc}}, \qquad \forall t, i, s \in I_t, c \in CT_t \tag{3.1}$$

where C^P_{tisc} and C^F_{tisc} are the respective concentrations of contaminant c in permeate and feed, for a technology, t, its pass, i and stage, s. R_{tisc} is the separation efficiency which can take values between 0, meaning no separation is accomplished, and 1, meaning 100% separation is attained. Thus, the extent of removal can be presented in the form of regression models based on Analysis of Variance (ANOVA), where the removal efficiencies are dependent variables, and the properties and operating conditions are independent variables. The correlations are readily found from laboratory experiments, modified or developed for the purpose of this study.

First, CF is considered where its removal efficiency for COD is determined by Eq. (3.2) [Sangeetha et al., 2014].

$$R_{tisc} = 0.00058 \cdot CD_{tis} + 0.135 \cdot pH_{tis} - 0.154, \qquad \forall t \in CF,\ i,s \in I_t,\ c \in COD \quad (3.2)$$

where CD_{tis} is the amount of coagulant and pH_{tis} is the concentration of hydrogen ions in the water. It is assumed CF has an insignificant effect in the removal of suspended solids, hence, its separation efficiency for this contaminant group is regarded as zero. The chemical dosage, the residence time and mixing in CF, however, effect the removal of TSS in the typically subsequent clarification processes, DAF and SED. Hence, when CLR is selected, CF also has to be selected. Additionally, if CLR is chosen, either SED's or DAF's removal ratio will be valid (Eq. (3.3)).

$$R_{tisc} = \sum_{q \in TCLR} \bar{R}_{qisc} \cdot X_{qis}, \qquad \forall t \in CLR,\ i,s \in I_t,\ c \in TSS \quad (3.3)$$

where X_{qis} is a binary variable for the selection of a clarification technology. It has been reported that sedimentation is strongly influenced by the coagulant dose used in CF [Vlaški, 1998]. After performing a regression analysis on the data provided in Vlaški [1998], the following correlation has been obtained:

$$\bar{R}_{qisc} = 0.22154 + 0.02516 \cdot CD_{tis}, \qquad \forall q \in SED,\ t \in CF,\ i,s \in I_t,\ c \in TSS \quad (3.4)$$

where CD_{tis} is the amount of coagulant used in the CF process. Besides coagulant dose, DAF also demonstrated dependence of detention time and velocity gradient in CF's mixing chamber, denoted as Tf_{tis} and Df_{tis}, respectively, in Eq. (3.5).

$$\bar{R}_{qisc} = 1.85886 - 0.00807 \cdot CD_{tis} - 0.00083 \cdot Gf_{tis} + 0.0025 \cdot Tf_{tis} - 2.47 \cdot \bar{P}_{qis},$$
$$\forall q \in DAF,\ t \in CF,\ i,s \in I_t,\ c \in TSS \quad (3.5)$$

where $\bar{P}_{qis}$ is the pressure of the saturator. The Commonwealth Scientific and Industrial

Research Organisation (CSIRO) developed the initial steady-state removal of TSS in media filtration (MMF) [Lin et al., 2006]. The relationship is shown in Eq. (3.6).

$$R_{tisc} = 0.0298 \cdot D^{MED}_{tis} + 0.171 \cdot Ld_{tis} + 0.206 \cdot L^{-1}_{tis} - 0.245, \quad \forall t \in MMF,\ i, s \in I_t,\ c \in TSS \tag{3.6}$$

where D^{MED}_{tis} stands for the diameter of the media, Ld_{tis} is the load to the filtration process, L^{-1}_{tis} is the length of the filter for MMF in pass i and stage s. The separation efficiency of COD from water by MF is shown in Eq. (3.7) derived from experimental work [Benitez et al., 2006].

$$R_{tisc} = 0.189 + 1.009 \cdot P_{tis}, \qquad \forall t \in MF,\ i, s \in I_t,\ c \in COD \tag{3.7}$$

The rejection of TSS by MF is affected by both pressure and temperature, thus:

$$R_{tisc} = 0.126 + 0.001 \cdot Tem_{tis} + 0.97 \cdot P_{tis}, \qquad \forall t \in MF,\ i, s \in I_t,\ c \in TSS \tag{3.8}$$

where Tem_{tis} is the temperature of the influent to technology t, pass i and stage s, and P_{tis} is the pressure of the feed flowrate. Cho et al. [2000] studied rejection of natural organic matter in UF membranes. Eq. (3.9) gives a regression where pressure is the only independent variable.

$$R_{tisc} = 0.236 - 0.952 \cdot P_{tis}, \qquad \forall t \in UF,\ i, s \in I_t,\ c \in COD \tag{3.9}$$

For the removal of turbidity by UF, Eq. (3.10) holds.

$$R_{tisc} = 0.959 - 1.510 \cdot P_{tis}, \qquad \forall t \in UF,\ i, s \in I_t,\ c \in TSS \tag{3.10}$$

where the equation has been derived from data obtained from pilot plant experimental work [Benitez et al., 2006].

Artug [2007] pointed out the NF membranes characteristics such as pore size, hydrophobicity and roughness affect their performance. Therefore, the retention for those membranes involves molecular weight cut-off, $MWCO_{tis}$, and hydrophobicity, H_{tis}, shown in Eq. (3.11) and Eq. (3.12).

$$R_{tisc} = 1.138 - 0.00096 \cdot MWCO_{tis} - 0.087 \cdot P_{tis}, \qquad \forall t \in NF,\, i, s \in I_t,\, c \in COD \tag{3.11}$$

$$R_{tisc} = (0.573 - 0.071 \cdot H_{tis} - 0.0002 \cdot MWCO_{tis})^2, \qquad \forall t \in NF,\, i, s \in I_t,\, c \in TDS \tag{3.12}$$

The correlation for TDS has been reported by Boussu et al. [2008] based on laboratory work. RO rejection coefficient for dissolved solids is presented in Eq. (3.13) as a function of the operating pressure performed on ROSA software [The Dow Chemical Company, 2013] by Chen and Guanghua [2005].

$$R_{tisc} = 0.890 + 0.034 \cdot P_{tis} - 0.003 \cdot P_{tis}^2, \qquad \forall t \in RO1,\, i, s \in I_t,\, c \in TDS \tag{3.13}$$

A separate contaminant group is dedicated to boron (B) which is detected in some water sources and its removal is particularly difficult due to its ionic dissolution [Li et al., 2008]. Consequently, elevated pH is necessary for its separation profile that can be modelled by Eq. (3.14).

$$R_{tisc} = 0.408 + 0.046 \cdot pH_{tis} + 0.028 \cdot P_{tis}, \qquad \forall t \in RO2,\, i, s \in I_t,\, c \in B \tag{3.14}$$

where pH_{tis} is the alkalinity of the solution to achieve desired separation. The above equation has been developed using ANOVA analysis and data from Mane et al. [2009].

Summary of separation coefficients

The regression equations described above and used in the model are summarised in Table 3.1.

TABLE 3.1: Summary of rejection coefficients correlations in MINLP model

Correlation		Equation
$R_{tisc} = 0.00058 \cdot CD_{tis} + 0.135 \cdot pH_{tis} - 0.154,$	$\forall t \in CF,\ i, s \in I_t,\ c \in COD$	(3.2)
$\bar{R}_{qisc} = 0.22154 + 0.02516 \cdot CD_{tis},$	$\forall q \in SED,\ t \in CF,\ i, s \in I_t,\ c \in TSS$	(3.4)
$\bar{R}_{qisc} = 1.85886 - 0.00807 \cdot CD_{tis} - 0.00083 \cdot Gf_{tis} + 0.0025 \cdot Tf_{tis} - 2.47 \cdot \bar{P}_{qis}$	$\forall q \in DAF,\ t \in CF,\ i, s \in I_t,\ c \in TSS$	(3.5)
$R_{tisc} = 0.0298 \cdot D_{tis}^{MED} + 0.171 \cdot Ld_{tis} + 0.206 \cdot L_{tis}^{-1} - 0.245,$	$\forall t \in MMF,\ i, s \in I_t,\ c \in TSS$	(3.6)
$R_{tisc} = 0.189 + 1.009 \cdot P_{tis},$	$\forall t \in MF,\ i, s \in I_t,\ c \in COD$	(3.7)
$R_{tisc} = 0.126 + 0.001 \cdot Tem_{tis} + 0.97 \cdot P_{tis},$	$\forall t \in MF,\ i, s \in I_t,\ c \in TSS$	(3.8)
$R_{tisc} = 0.236 - 0.952 \cdot P_{tis},$	$\forall t \in UF,\ i, s \in I_t,\ c \in COD$	(3.9)
$R_{tisc} = 0.959 - 1.510 \cdot P_{tis},$	$\forall t \in UF,\ i, s \in I_t,\ c \in TSS$	(3.10)
$R_{tisc} = 1.138 - 0.00096 \cdot MWCO_{tis} - 0.087 \cdot P_{tis},$	$\forall t \in NF,\ i, s \in I_t,\ c \in COD$	(3.11)
$R_{tisc} = (0.57 - 0.07 \cdot H_{tis} - 0.0002 \cdot MWCO_{tis})^2,$	$\forall t \in NF,\ i, s \in I_t,\ c \in TDS$	(3.12)
$R_{tisc} = 0.890 + 0.0340 \cdot P_{tis} - 0.003 \cdot P_{tis}^2,$	$\forall t \in RO1,\ i, s \in I_t,\ c \in TDS$	(3.13)
$R_{tisc} = 0.408 + 0.046 \cdot pH_{tis} + 0.028 \cdot P_{tis},$	$\forall t \in RO2,\ i, s \in I_t,\ c \in B$	(3.14)

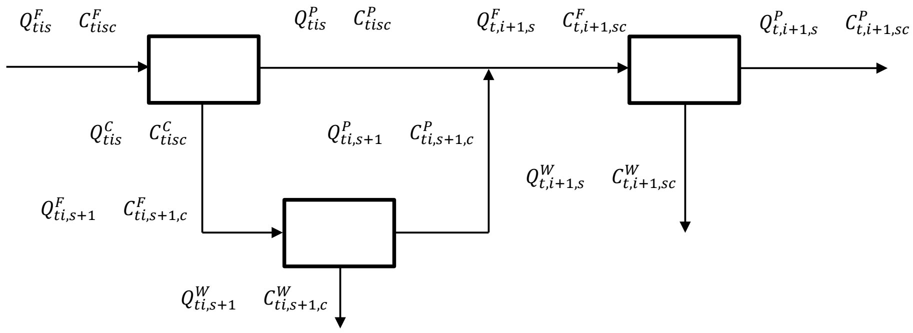


FIGURE 3.2: A schematic representation of concentrations and flows streams in a two-pass system with two and one stages

3.3.1.2 Mass balance constraints

Next, the concentration and mass balances constraints are presented. A simple schematic representation of feed, permeate, concentrate and waste streams is depicted in Fig. 3.2.

Concentration constraints

The permeate concentrations, C^P_{tisc}, of every unit are calculated in Eq. (3.15) and Eq. (3.16). If a unit is selected, its concentration is reduced to C^P_{tisc}. Otherwise, the concentration remains C^F_{tisc}.

$$C^F_{tisc} \cdot (1 - R_{tisc}) - M^{BIG}_c \cdot (1 - E_{tis}) \leq C^P_{tisc} \leq C^F_{tisc} \cdot (1 - R_{tisc}) + M^{BIG}_c \cdot (1 - E_{tis}),$$
$$\forall t, i, s \in I_t, c \in CT_t \tag{3.15}$$

$$C^F_{tisc} - M^{BIG}_c \cdot E_{tis} \leq C^P_{tisc} \leq C^F_{tisc}, \qquad \forall t, i, s \in I_t, c \in CT_t \tag{3.16}$$

where M^{BIG}_c is a big number with a unique value for every c. M^{BIG}_c should be adjusted for every contaminant because of the difference in concentrations magnitudes. E_{tis} is a binary variable which is activated when a technology t, pass i and stage s are selected. Eq. (3.15) involves a bilinear product of C^F_{tisc} and R_{tisc}. When a unit is selected, then the retentate concentrations, C^C_{tisc}, would either equate waste concentrations, C^W_{tisc}, or the feed concentrations of the next stage (Eq. (3.17) - Eq. (3.19)). The expressions are valid only for the contaminants relevant for a technology.

$$C^C_{ti,s-1,c} = C^F_{tisc} + C^W_{ti,s-1,c}, \qquad \forall t, i, s \in I_t, s > 1, c \in CT_t \tag{3.17}$$

If a next stage is not selected, the stream goes to waste which can be further diluted or treated, or discharged.

$$C^W_{ti,s-1,c} \leq M^{BIG}_c \cdot (1 - E_{tis}), \qquad \forall t, i, s \in I_t, s > 1, c \in CT_t \tag{3.18}$$

If a next stage is chosen, the effluent from the previous stage becomes the feed of the next stage.

$$C^F_{tisc} \leq M^{BIG}_c \cdot E_{tis}, \qquad \forall t, i, s \in I_t, s > 1, c \in CT_t \tag{3.19}$$

In order to ensure no value will be given to the concentrates when a stage is not selected, we enforce the following constraint:

$$C^C_{tisc} \leq M^{BIG}_c \cdot E_{tis}, \qquad \forall t, i, s \in I_t, c \in CT_t \tag{3.20}$$

where M^{BIG} is sufficiently large so that it will always be greater than the concentration of the concentrate. Furthermore, we would like to ensure the contaminants that cannot be treated by a technology would have a zero value for their waste concentration:

$$C^C_{tisc} = 0, \qquad \forall t, i, s \in I_t, c \notin CT_t \tag{3.21}$$

Flowrate constraints

Similarly, the flowrate constraints are modelled in Eq. (3.22) and Eq. (3.23). When a candidate is selected, the feed Q^F_{tis} is reduced to Q^P_{tis}.

$$\begin{aligned} y_{tis} \cdot Q^F_{tis} - Q^{IN} \cdot (1 - E_{tis}) \leq Q^P_{tis} \leq y_{tis} \cdot Q^F_{tis} + Q^{IN} \cdot (1 - E_{tis}), \\ \forall t \notin CLR,\ i, s \in I_t \end{aligned} \tag{3.22}$$

$$Q^F_{tis} - Q^{IN} \cdot E_{tis} \leq Q^P_{tis} \leq Q^F_{tis}, \qquad \forall t \notin CLR,\ i, s \in I_t \tag{3.23}$$

where y_{tis} is the recovery of a technology t, pass i and stage s. Although unit recovery, like removal efficiency, can also be expressed as a function of the system pressure, fluid salinity, etc. [Li et al., 2008], in this work the recoveries are modelled as parameters which take different values for every t. Q^{IN} is the intake flowrate and serves a purpose of an upper bound of the product flow. Q^P_{tis} and Q^F_{tis} are the permeate and feed flowrates, respectively, associated with a technology t, pass i and stage s. As previously mentioned, SED and DAF are represented by CLR, whose flowrate is determined either by the recovery value of SED or the recovery value of DAF (Eq. (3.24)).

$$Q^P_{tis} = Q^F_{tis} \cdot \sum_{q \in TCLR} (\bar{y}_{qis} \cdot X_{qis}) + Q^F_{tis} \cdot (1 - \sum_{q \in TCLR} X_{qis}), \quad \forall t \in CLR,\ i, s \in I_t \tag{3.24}$$

In the cases where there are more than one stage selected, the concentrate flow, Q^C_{tis} from the previous stage equals the feed flow of the next stage (Eq. (3.25)).

$$Q^C_{ti,s-1} = Q^F_{tis} + Q^W_{ti,s-1}, \qquad \forall t, i, s \in I_t, s > 1 \tag{3.25}$$

$$Q^F_{tis} \leq Q^{IN} \cdot E_{tis}, \qquad \forall t, i, s \in I_t, s > 1 \tag{3.26}$$

If a next stage is not selected, the value of the concentrate flow will be passed to a waste stream Q^W_{tis}.

$$Q^W_{ti,s-1} \leq Q^{IN} \cdot (1 - E_{tis}), \qquad \forall t, i, s \in I_t, s > 1 \tag{3.27}$$

In order to ensure no flow is passed to the waste stream when a stage is not selected, the following constraint is applied:

$$Q^C_{tis} \leq Q^{IN} \cdot E_{tis}, \qquad \forall t, i, s \in I_t \tag{3.28}$$

When the flows are passed from one pass to another, Eq. (3.29) holds.

$$\sum_{s \in I_t} Q^P_{t,i-1,s} = Q^F_{tis|s=1}, \qquad \forall t, i \in I_t, i > 1 \tag{3.29}$$

When the flows are passed from one technology to another, Eq. (3.30) is used.

$$\sum_{s \in I_t} Q^P_{t-1,is|i=I_t^{max}} = Q^F_{tis|i=1,s=1}, \qquad \forall t > 1 \tag{3.30}$$

Balances and interconnections constraints

The mass and concentration balances over a pass and a stage are expressed in Eq. (3.31) - Eq. (3.32).

$$C^{C}_{tisc} \cdot Q^{C}_{tis} = C^{F}_{tisc} \cdot Q^{F}_{tis} - C^{P}_{tisc} \cdot Q^{P}_{tis}, \qquad \forall t, i, s \in I_t, c \tag{3.31}$$

$$Q^{C}_{tis} = Q^{F}_{tis} - Q^{P}_{tis}, \qquad \forall t, i, s \in I_t \tag{3.32}$$

The interconnection between two passes is expressed in Eq. (3.33) and the interconnection between two technologies is expressed in Eq. (3.34).

$$\sum_{s \in I_t} C^{P}_{t,i-1,sc} \cdot Q^{P}_{t,i-1,s} = C^{F}_{tisc|s=1} \cdot Q^{F}_{tis|s=1}, \qquad \forall t, i \in I_t, i > 1, c \tag{3.33}$$

$$\sum_{s \in I_t} C^{P}_{t-1,isc|i=I^{max}_t} \cdot Q^{P}_{t-1,is|i=I^{max}_t} = C^{F}_{tisc|i=1,s=1} \cdot Q^{F}_{tis|i=1,s=1}, \qquad \forall t > 1, c \tag{3.34}$$

The hourly, $Qout$, and annual, Q^{AP}, production rates of the facility are then expressed by Eq. (3.35) and Eq. (3.36), respectively.

$$Qout = \sum_{s \in I_t} Q^{P}_{tis}, \qquad \forall t = T,\ i = I^{max}_t \tag{3.35}$$

$$Q^{AP} = t_h \cdot t_d \cdot py \cdot Qout \tag{3.36}$$

where t_h is the number of operating hours per day, t_d is the number of operating days per year and py is the production fraction of the facility relative to its capacity.

3.3.1.3 Target constraints

The final contaminant concentrations, $Cout_c$, should satisfy the conditions imposed by Eq. (3.37) and Eq. (3.38) and do not exceed the maximum allowable concentration, M^{CONC}_c. The final purity requirements alter with the ultimate purpose of the product, i.e. drinking water, process water, water for irrigation.

$$Cout_c \cdot Qout = \sum_{s \in I_t} (C^{P}_{tisc} \cdot Q^{P}_{tis}), \qquad \forall t = T, i = I^{max}_t, c \tag{3.37}$$

$$Cout_c \leq M_c^{CONC}, \qquad \forall c \tag{3.38}$$

A supplementary constraint for minimum effluent amount is enforced by Eq. (3.39) which would ensure the plant design capacity is met.

$$Qout \geq M^{FLOW} \tag{3.39}$$

where M^{FLOW} is the minimum allowable effluent flow.

3.3.1.4 Logical constraints

The overall number of the selected technologies, passes and stages should not be greater than a number, N^{max}, shown in Eq. (3.40).

$$\sum_t \sum_{i \in I_t} \sum_{s \in I_t} E_{tis} \leq N^{max} \tag{3.40}$$

Eq. (3.41) and Eq. (3.42) are logical conditions that do not allow the selection of any pass or stage provided the previous one has not been chosen.

$$E_{t,i+1,s} \leq E_{tis}, \qquad \forall t, i, s \in I_t, i+1 \in I_t \tag{3.41}$$

$$E_{ti,s+1} \leq E_{tis}, \qquad \forall t, i, s \in I_t, s+1 \in I_t \tag{3.42}$$

Coagulation-flocculation should be selected when sedimentation or dissolved air flotation is selected hence, Eq. (3.43) applies:

$$E_{qis} \leq E_{tis}, \qquad \forall q \in CLR, t \in CF, i = 1, s = 1 \tag{3.43}$$

Only one of the clarification processes can be chosen at a time, a condition imposed by Eq. (3.44).

$$\sum_{q \in TCLR} X_{qis} = E_{tis}, \qquad \forall t \in CLR, i, s \in I_t \tag{3.44}$$

The same logical conditions for binary variable X_{qis} are needed.

$$X_{q,i+1,s} \leq X_{qis}, \qquad \forall q, i, s \in \bar{I}_q, i+1 \in \bar{I}_q \tag{3.45}$$

$$X_{qi,s+1} \leq X_{qis}, \qquad \forall q, i, s \in \bar{I}_q, s+1 \in \bar{I}_q \tag{3.46}$$

3.3.1.5 Cost constraints

Economic appraisal of conceptual design owes its complexity to the various cost components that must be considered. Such components are plant capacity, intake quality and quantity, location, accessibility to electricity and occurring electricity charges, qualified labour, plant life, agreements with banks and local governments [Zhou and Tol, 2004]. In the following subsections, many of the factors have been included such as chemical costs for coagulant, pH adjustments and post-treatment, electricity for mixing and pumping, equipment replacement and labour. No carbon taxation is assumed.

3.3.1.5.1 Operating costs Aluminium sulphate (alum) and ferric sulphate are the preferred choice of coagulants where the former is widely used in surface water treatment due to its low cost and the latter is a more common choice in desalination because of its better performance. The annual cost for the chemical requirements is calculated from Eq. (3.47).

$$CHC_{tis} = cv^{CHC} \cdot t_h \cdot t_d \cdot c^{chem} \cdot CD_{tis} \cdot Q^{FL}_{tis}, \qquad \forall t \in CF, i, s \in I_t \tag{3.47}$$

where cv^{CHC} is a conversion factor, t_d is the number of operating days a year, t_h is the number of operating hours a day, CD_{tis} is the coagulant dose and c^{chem} is the cost of coagulant. Q^{FL}_{tis} is the linearised flowrate of a bilinear term for the multiplication of the feed flowrate and the binary variable E_{tis}. The term is determined by Eqs. (3.48) and (3.49).

$$Q^{FL}_{tis} \leq Q^{IN} \cdot E_{tis}, \qquad \forall t, i, s \in I_t \tag{3.48}$$

$$Q^{F}_{tis} - Q^{IN} \cdot (1 - E_{tis}) \leq Q^{FL}_{tis} \leq Q^{F}_{tis} + Q^{IN} \cdot (1 - E_{tis}), \qquad \forall t, i, s \in I_t \tag{3.49}$$

The linearised term is used in calculating the electricity cost for the slow mixing in the flocculant tank (Eq. (3.50)).

$$EMC_{tis} = cv^{EM} \cdot t_d \cdot t_h \cdot \mu \cdot c^{E} \cdot Tf_t \cdot Q^{FL}_{tis} \cdot Gf^2_{tis}, \forall t \in CF, i, s \in I_t \tag{3.50}$$

In Eq. (3.50), cv^{EM} is conversion factor, μ is the dynamic viscosity of the fluid and c^E is the electricity charge. The ongoing costs for DAF depend mainly on its saturator which is expressed in Eq. (3.51).

$$SC_{tis} = \frac{cv^{SC} \cdot c^E \cdot \bar{P}_{qis} \cdot Q^F_{tis} \cdot X_{qis}}{\eta^{SAT}}, \qquad \forall t \in CLR, q \in DAF, i, s \in I_t \tag{3.51}$$

where SC_{tis} is the operating cost of the saturator, cv^{SC} is the conversion factor for the equation, η_t^{SAT} is the efficiency of the saturator, $\bar{P_{qis}}$ is the saturator pressure, assumed to be the pressure supplied by the pump and c^E is the electricity cost rate. The most significant contribution to the operating costs stems from electricity, and more specifically, electricity for flowrates distribution and achieving separation pressure. Hence, the feed pumps are the main electricity consumers and their costs, denoted as PC_{tis}, are expressed in the following equation.

$$PC_{tis} = \frac{cv^{PC} \cdot c^E \cdot P_{tis} \cdot Q^{FL}_{tis}}{\eta_t^{FP} \cdot \eta_t^{MT}}, \qquad \forall t \notin CLR, i, s \in I_t \tag{3.52}$$

cv^{PC} is a conversion factor for the pumping cost equation. No pumps are assigned to the clarification processes in order to avoid breaking the flocs formed in CF.

The replacement costs, MRC_{tis}, are estimated for every pass i and stage s. For media filtration, they will depend on the volume of media to be purchased.

$$MRC_{tis} = af^{MRC} \cdot rc_t^M \cdot \frac{\pi \cdot L_{tis} \cdot D^{MED^2}_{tis}}{4} \cdot E_{tis} \qquad \forall t \in MMF, i, s \in I_t \tag{3.53}$$

For membrane filtration, the replacement cost is governed by the permeate flowrate:

$$MRC_{tis} = af^{MRC} \cdot t_h \cdot t_d \cdot rc_t^M \cdot y_{tis} \cdot Q^{FL}_{tis} \qquad \forall t \in TMM, i, s \in I_t \tag{3.54}$$

where af^{MRC} is an annualisation factor allowing membrane life of 5 years and rc^M is the membrane replacing cost per cubic metre media purchased (for media filtration) or permeate produced (for membrane filtration). It is assumed that the lifespan of the chambers for CF, SED and DAF lasts as long as the plant's life. The chemical costs for pH adjusting, treatment and post-treatment can also be expressed in terms of the capacity of the plant, hence:

$$ChemC = t_h \cdot t_d \cdot py \cdot r^{ch} \cdot Qout \tag{3.55}$$

where r^{ch} is the cost for chemicals per volume of produced water.

The labour cost, LC, accounts for another large ongoing expense in a manufacturing facility. It can be estimated based on the production capacity of the plant, as shown in Eq. (3.56).

$$LC = lc1 \cdot Qout + lc2 \tag{3.56}$$

where $lc1$ and $lc2$ are, respectively, the coefficient and intercept of the linear dependency of daily plant capacity and annual labour cost.

3.3.1.5.2 Capital costs Capital costs for every plant are comprised of four major components, namely, project development, plant equipment and buildings, power supply, and piping and pumps [Blaikie et al., 2013]. An estimation of the capital cost, however, can be given by the capacity for water production and thus, the following expression can be used:

$$CC_{tis} = infl_t \cdot A_t \cdot (Q^P_{tis})^{b_t} \cdot E_{tis}, \qquad \forall t \notin CLR, i, s \in I_t \tag{3.57}$$

where $infl_t$ is inflation factor depending on the year of estimation, A_t and b_t are specific parameters for every technology. The capital cost for the clarification technologies is calculated from Eq. (3.58).

$$CC_{tis} = \sum_{q \in TCLR} infl_q \cdot A_q \cdot (Q^P_{tis})^{b_q} \cdot X_{qis}, \qquad \forall t \in CLR, i, s \in I_t \tag{3.58}$$

The capital recovery factory (CRF) is expressed in Eq. (3.59) [Badiru and Omitaomu, 2007].

$$CRF = \frac{ir}{1 - \frac{1}{(1+ir)^{yr}}} \tag{3.59}$$

where ir is the bank interest rate and yr is the number of years for investment which often coincides with the plant life.

3.3.1.5.3 Total cost The total annual cost, TC, is a sum of the coagulant CHC_{tis}, mixing EMC_{tis}, saturator SC_{tis}, pumping PC_{tis}, replacement MRC_{tis}, chemical conditioning $ChemC$, labour LC and the annual capital costs for all the selected technologies.

$$\begin{aligned}
TC = & \sum_{t\in CF}\sum_{i\in I_t}\sum_{s\in I_t} CHC_{tis} + ChemC + && \text{chemical costs}\\
& \sum_{t\in CF}\sum_{i\in I_t}\sum_{s\in I_t} EMC_{tis} + \sum_{t\in CLR}\sum_{i\in I_t}\sum_{s\in I_t} SC_{tis} + \sum_{t\notin CLR}\sum_{i\in I_t}\sum_{s\in I_t} PC_{tis} + && \text{power costs}\\
& \sum_{t\in TMMB}\sum_{i\in I_t}\sum_{s\in I_t} MRC_{tis} + && \text{replacement cost}\\
& LC + && \text{labour cost}\\
& \sum_{t}\sum_{i\in I_t}\sum_{s\in I_t} CRF \cdot CC_{tis} && \text{capital cost}
\end{aligned} \tag{3.60}$$

3.3.1.6 Objective function

The objective function for the MINLP model is to minimise the water net cost, WNC, which is the quotient of the total annual cost and the annual plant production rate:

$$minimise \quad WNC = \frac{TC}{Q^{AP}} \tag{3.61}$$

which is subject to:

- separation efficiencies Eq. (3.2) - Eq. (3.14)
- mass balances Eq. (3.15) - Eq. (3.36)
- targets Eq. (3.37) - Eq. (3.39)
- logical conditions Eq. (3.40) - Eq. (3.46)
- operating costs Eq. (3.47) - Eq. (3.56)
- capital costs Eq. (3.57) - Eq. (3.58)
- total annual cost Eq. (3.60)

While minimising the annualised capital investment and running costs, the annual production flowrate is increased and the optimum purity is achieved. Nevertheless, the formulation contains various non-linearities that result in multiple local minima. In pursuit for better model stability, the most abundant non-linearities generated from mass balance constraints are reformulated, together with the capital cost function which is demonstrated in the next subsection.

3.3.2 Partially linearised MINLP (plMINLP) model formulation (P1)

The model presented in Section 3.3.1 is highly non-linear and its convergence is challenging, resulting in many cases in infeasible solutions. Accordingly, the model has been linearised. The constraints related to mass balances (Eqs. (3.31), (3.33), (3.34) and (3.37)) and economies of scale (Eqs. (3.58) and (3.59)) were initially reformulated. The relaxation and piecewise approximation procedures are presented in the following sections.

3.3.2.1 Mass balances linearisations

The bilinear terms $C^P_{tisc} \cdot Q^P_{tis}$, $C^F_{tisc} \cdot Q^F_{tis}$, $C^C_{tisc} \cdot Q^C_{tis}$ arising from the multiplication of two continuous variables, i.e. contaminants and flowrates, in Eqs. (3.31), (3.33) and (3.34) were reformulated using multiparametric disaggregation [Teles et al., 2012, Kolodziej et al., 2013, Teles et al., 2013, Castro, 2016] where the flowrate is expressed as a multiparametric sum of active decimal powers determined by binary variables z_{tisckl} and continuous variables $\bar{z}_{tisck}$, and the concentrations variable is disaggregated into a set of continuous non-negative variables $\hat{C}_{tisckl}$ and $\bar{C}_{tisck}$. The variables are with superscripts corresponding to the stream they belong to, i.e. permeate, feed and concentrate. Thus, the reformulation for permeate, for instance, becomes:

$$CQ^P_{tisc} = \sum_{l=p}^{P}\sum_{k=0}^{9} 10^l \cdot k \cdot \hat{C}^P_{tisckl} + \sum_{k=0}^{1} 10^p \cdot k \cdot \bar{C}^P_{tisck}, \qquad \forall t, i, s \in I_t, c \tag{3.62}$$

where $k = \{0, 1, 2, ..., 9\}$. The flowrate is represented in Eq. (3.63) where the second term provides fine tuning and hence, continuity in the domain of the flowrate.

$$Q^P_{tis} = \sum_{l=p}^{P}\sum_{k=0}^{9} 10^l \cdot k \cdot zp_{tisckl} + \sum_{k=0}^{1} 10^p \cdot k \cdot \bar{z}p_{tisck}, \qquad \forall t, i, s \in I_t, c \tag{3.63}$$

The newly introduced non-negative continuous variables $\hat{C}^P_{tisckl}$ and $\bar{C}^P_{tisck}$ are bounded by M^{BIG}_c or zeroed depending on the value the binary and pseudo-binary variables will take.

$$\hat{C}^P_{tisckl} \leq M^{BIG}_c \cdot zp_{tisckl}, \qquad \forall t, i, s \in I_t, c, k, l \tag{3.64}$$

$$\bar{C}^P_{tisck} \leq M^{BIG}_c \cdot \bar{z}p_{tisck}, \qquad \forall t, i, s \in I_t, c, k \leq 1 \tag{3.65}$$

Eq. (3.66) and Eq. (3.67) relate $\hat{C}^P_{tisckl}$ and $\bar{C}^P_{tisck}$ with the variable C^P_{tisc} additional constraints are introduced.

$$\sum_{k=0}^{9} \hat{C}^P_{tisckl} = C^P_{tisc}, \qquad \forall t, i, s \in I_t, c, l \tag{3.66}$$

$$\sum_{k=0}^{1} \bar{C}^P_{tisck} = C^P_{tisc}, \qquad \forall t, i, s \in I_t, c \tag{3.67}$$

The selection of only one variable over the k set is imposed by Eq. (3.68) and Eq. (3.69).

$$\sum_{k=0}^{9} zp_{tisckl} = 1, \qquad \forall t, i, s \in I_t, c, l \tag{3.68}$$

$$\sum_{k=0}^{1} \bar{z}p_{tisck} = 1, \qquad \forall t, i, s \in I_t, c \tag{3.69}$$

The continuous variable $\bar{z}p_{tisck}$ is bounded between 0 and 1. The feed and concentrate have been reformulated using the same method where superscripts F and C were used to designate the respective variables. Replacing the bilinear products, transforms Eq. (3.31) to the following constraint:

$$CQ^C_{tisc} = CQ^F_{tisc} - CQ^P_{tisc}, \qquad \forall t, i, s \in I_t, c \tag{3.70}$$

Eq. (3.33) and Eq. (3.34) acquire the form, shown in Eq. (3.71) and Eq. (3.72).

$$\sum_{s \in I_t} CQ^P_{t,i-1,sc} = CQ^F_{tisc|s=1}, \qquad \forall t, i \in I_t, i > 1, c \tag{3.71}$$

$$\sum_{s \in I_t} CQ^P_{t-1,isc|i=I^{max}_t} = CQ^F_{tisc|i=1,s=1}, \qquad \forall t > 1, c \tag{3.72}$$

The bilinear terms arising from the multiplication of continuous variables of contaminant levels and flowrates for final effluent in Eq. (3.37) were reformulated in a similar manner, demonstrated below.

$$CQout_c = \sum_{l=p}^{P} \sum_{k=0}^{9} 10^l \cdot k \cdot C\hat{o}ut_{ckl} + \sum_{k=0}^{1} 10^p \cdot k \cdot C\bar{o}ut_{ck}, \qquad \forall c \tag{3.73}$$

where $C\hat{o}ut_{ckl}$ and $C\bar{o}ut_{ck}$ are the auxiliary continuous variables to represent final concentrations. The effluent is expressed as a summation of two terms where zo_{ckl} is a binary variable and $\bar{zo}_{ck}$ a continuous variable, both to determine the selection of a single digit number k and decimal number raised to power l.

$$Qout = \sum_{l=p}^{P} \sum_{k=0}^{9} 10^l \cdot k \cdot zo_{ckl} + \sum_{k=0}^{1} 10^p \cdot k \cdot \bar{zo}_{ck}, \qquad \forall c \tag{3.74}$$

$C\hat{o}ut_{ckl}$ and $C\bar{o}ut_{ck}$ are bounded by a big number in the following constraints.

$$C\hat{o}ut_{ckl} \leq M_c^{BIG} \cdot zo_{ckl}, \qquad \forall c, k, l \tag{3.75}$$

$$C\bar{o}ut_{ck} \leq M_c^{BIG} \cdot \bar{zo}_{ck}, \qquad \forall c, k \leq 1 \tag{3.76}$$

$C\hat{o}ut_{ckl}$ and $C\bar{o}ut_{ck}$ and $Cout_c$ are related in Eq. (3.77) and Eq. (3.78).

$$\sum_{k=0}^{9} C\hat{o}ut_{ckl} = Cout_c, \qquad \forall c, l \tag{3.77}$$

$$\sum_{k=0}^{1} C\bar{o}ut_{ck} = Cout_c, \qquad \forall c \tag{3.78}$$

Only the selection of one significant digit for every power is possible:

$$\sum_{k=0}^{9} zo_{ckl} = 1, \qquad \forall c, l \tag{3.79}$$

$$\sum_{k=0}^{1} \bar{zo}_{ck} = 1, \qquad \forall c \tag{3.80}$$

The continuous variable $\bar{zo}_{ck}$ is between 0 and 1. Because permeate, feed, concentrate and final flowrates are in the same order of magnitude, the power they are raised to is the same. The bilinear products are now substituted in Eq. (3.37) and it is remodelled to Eq. (3.81).

$$CQ_{out_c} = \sum_{s \in I_t} CQ^P_{tisc}, \qquad \forall t = T, i = I_t^{max}, c \tag{3.81}$$

3.3.2.2 Approximation of capital cost constraints

The capital cost is represented by a piecewise linear approximation, defined over the domain of the flowrate. Taking Q^{IN} as an initial point and M^{FLOW} as a final point in this domain, the optimal number of segments and connecting points are obtained with the approach published in Natali and Pinto [2009]. The function from Eq. (3.57) and Eq. (3.58) is expressed through cco^{bp}_{tism} and q^{pbp}_{tism}, parameters representing segments m of the cost and flowrate, respectively, in Eq. (3.82).

$$cco^{bp}_{tism} = infl_t \cdot A_t \cdot (q^{pbp}_{tism})^{b_t}, \qquad \forall t \notin CLR, i, s \in I_t, m \tag{3.82}$$

where $infl_t$ is inflation factor depending on the year of estimation, A_t and b_t are specific parameters for every technology. Similar to the formulation in the previous subsection, the cost function of the clarification processes is calculated separately:

$$cco^{bp}_{qism} = infl_q \cdot A_q \cdot (q^{pbp}_{qism})^{b_q}, \qquad \forall q \in TCLR, i, s \in \bar{I}_q, m \tag{3.83}$$

The performed piecewise approximation is shown below where G_{tism} is a continuous variable and Y^m_{tism} is a binary variable.

$$Q^P_{tis} = \sum_m (q^{pbp}_{tism} \cdot G_{tism}), \qquad \forall t \notin CLR, i, s \in I_t \tag{3.84}$$

Eq. (3.85) connects the flowrate of CLR with the properties of SED and DAF:

$$Q^P_{tis} = \sum_m (q^{pbp}_{qism} \cdot G_{qism}), \qquad \forall t \in CLR, q \in TCLR, i, s \in I_t \tag{3.85}$$

The capital cost $CCol_{tis}$ is related in Eq. (3.86) and Eq. (3.87).

$$CCol_{tis} = \sum_m (cco^{bp}_{tism} \cdot G_{tism}), \qquad \forall t \notin CLR, i, s \in I_t \tag{3.86}$$

$$CCol_{qis} = \sum_m (cco^{bp}_{qism} \cdot G_{qism}), \qquad \forall q \in TCLR, i, s \in \bar{I}_q \tag{3.87}$$

Only one segment m for a given technology t, pass i and stage s is allowed (Eq. (3.88)).

$$\sum_m G_{tism} = 1, \qquad \forall t, i, s \in I_t \tag{3.88}$$

$$G_{tism} \leq Y^m_{tis,m-1} + Y^m_{tism}, \qquad \forall t, i, s \in I_t, m < M^{max} - 1 \tag{3.89}$$

$$\sum_{m<M^{max}-1} Y^m_{tism} = 1, \qquad \forall t, i, s \in I_t \tag{3.90}$$

Standard piecewise linearisation technique utilising one continuous and one discrete variables instead of SOS2 variables is implemented as SOS variables are not supported by most global non-linear solvers. In order to consider the cost only for the selected units, a bilinear term will appear which has to be linearised. Thus, for non clarification technologies:

$$CC_{tis} \leq U^{BIG}_t \cdot E_{tis}, \qquad \forall t \notin CLR, i, s \in I_t \tag{3.91}$$

$$CCol_{tis} - U^{BIG}_t \cdot E_{tis} \leq CC_{tis} \leq CCol_{tis} + U^{BIG}_t \cdot E_{tis}, \qquad \forall t \notin CLR, i, s \in I_t \tag{3.92}$$

where U^{BIG}_t is a sufficiently big number. The presence or absence of capital cost for CLR rests on the value of the binary variable X_{qis} which can take the value of 1 either for SED or for DAF only.

$$CC_{tis} \leq U^{BIG}_q \cdot X_{qis}, \qquad \forall t \in CLR, q \in TCLR, i, s \in I_t \tag{3.93}$$

$$\begin{aligned} CCol_{qis} - U^{BIG}_q \cdot (1 - X_{qis}) \leq CC_{tis} \leq CCol_{qis} + U^{BIG}_q \cdot (1 - X_{qis}), \\ \forall t \in CLR, q \in TCLR, i, s \in I_t \end{aligned} \tag{3.94}$$

3.3.2.3 Objective function

The objective function for the plMINLP model is to minimise the water net cost, WNC, which equals the total annual cost divided by the annual plant production rate:

$$minimise \quad WNC = \frac{TC}{Q^{AP}}$$

which is subject to:

- separation efficiencies Eq. (3.2) - Eq. (3.14)
- mass balances Eq. (3.15) - Eq. (3.30), Eqs. (3.32), Eq. (3.35),Eq. (3.36), Eq. (3.62) - Eq. (3.72)
- targets Eq. 3.38, Eq. (3.39), Eq. (3.73) - Eq. (3.81)
- logical conditions Eq. (3.40) - Eq. (3.46)

- operating costs Eq. (3.47) - Eq. (3.56)
- capital costs Eq. (3.84) - Eq. (3.94)
- total annual cost Eq. (3.60)

An alternative formulation can be obtained if $P1$ is completely linearised.

3.3.3 MILP model formulation (P2)

The model presented in Section 3.3.2 can be linearised completely to enhance robustness. Although a linear model is only an approximation to the original problem, the linearisation of the model guarantees a convex approximation which greatly benefits the convergence. Eqs. (3.2) - (3.14) contain regressions which are not only linear but also quadratic, logarithmic and reciprocal. Due to the different nature of non-linearities, discretisation of the physicochemical properties and operating conditions are performed. Additionally, the running costs, that also contain operating conditions (Eqs. (3.47), (3.50), (3.51), (3.52) and (3.53)), are also reformulated. Finally, it is desirable to increase the throughput of the flowsheet, hence, Q^{AP} remains a variable and the model becomes fractional. For the purpose of tackling with the non-linearity, a variation of the Dinkelbach's algorithm is implemented as a solution approach to the ratio in the objective function in Eq. (4.61).

3.3.3.1 Rejection coefficient discretisations

The separation efficiencies have been discretised to avoid the nonlinearities in Eq. (3.2) - Eq. (3.14). A subscript j denotes the levels of discretisations of both, the separation efficiencies and operating conditions, which vary with the technologies. The form the correlations take is summarised in Table 3.2 where r_{tcj} is the separation efficiency of every technology t and contaminant c and at a discrete level j. Furthermore, the equations differ from the correlations in Section 3.3.1 with the terms being declared as parameters and denoted with small letters, and the additional index.

TABLE 3.2: Summary of rejection coefficients correlations in MILFP model

Correlation		Equation
$r_{tcj} = 0.00058 \cdot cd_{tj} + 0.135 \cdot ph_{tj} - 0.154,$	$\forall t \in CF, c \in COD, j \in J_t$	(3.95)
$rq_{tqcj} = 0.22154 + 0.02516 \cdot cd_{tj\|t=CF},$	$\forall t \in CLR, q \in SED,\ c \in TSS, j \in J_t$	(3.96)
$rq_{tqcj} = 1.85886 - 0.00807 \cdot cd_{tj\|t=CF} - 0.00083 \cdot gf_{tj\|t=CF} +$ $0.0025 \cdot tf_{tj\|t=CF} - 2.47 \cdot \bar{p}_{qj},$	$\forall t \in CLR, q \in DAF, c \in TSS, j \in J_t$	(3.97)
$r_{tcj} = 0.0298 \cdot d_{tj}^{MED} + 0.171 \cdot ld_{tj} + 0.206 \cdot l_{tj}^{-1} - 0.245,$	$\forall t \in MMF, c \in TSS, j \in J_t$	(3.98)
$r_{tcj} = 0.189 + 1.009 \cdot p_{tj},$	$\forall t \in MF, c \in COD, j \in J_t$	(3.99)
$r_{tcj} = 0.126 + 0.001 \cdot tem_{tj} + 0.97 \cdot p_{tj},$	$\forall t \in MF, c \in TSS, j \in J_t$	(3.100)
$r_{tcj} = 0.236 - 0.952 \cdot p_{tj},$	$\forall t \in UF,\ c \in COD, j \in J_t$	(3.101)
$r_{tcj} = 0.959 - 1.510 \cdot p_{tj},$	$\forall t \in UF, c \in TSS, j \in J_t$	(3.102)
$r_{tcj} = 1.138 - 0.00096 \cdot mwco_{tj} - 0.087 \cdot pj_{tj},$	$\forall t \in NF, c \in COD, j \in J_t$	(3.103)
$r_{tcj} = (0.57 - 0.07 \cdot h_{tj} - 0.0002 \cdot mwco_{tj})^2,$	$\forall t \in NF, c \in TDS, j \in J_t$	(3.104)
$r_{tcj} = 0.890 + 0.0340 \cdot p_{tj} - 0.003 \cdot p_{tj}^2,$	$\forall t \in RO1, c \in TDS, j \in J_t$	(3.105)
$r_{tcj} = 0.408 + 0.046 \cdot ph_{tj} + 0.028 \cdot p_{tj},$	$\forall t \in RO2, c \in B, j \in J_t$	(3.106)

The selection of the rejection coefficient is expressed through a binary variable, W_{tisj}, which designates if an combinatorial option from the given operating conditions is selected or not.

$$R_{tisc} = \sum_{j \in J_t} r_{tcj} \cdot W_{tisj}, \qquad \forall t \notin CLR, i, s \in I_t, c \in CT_t \tag{3.107}$$

Then, the discrete levels selected, should equal the binary variable E_{tis}, shown in Eq. (3.108).

$$\sum_{j \in J_t} W_{tisj} = E_{tis}, \qquad \forall t \notin CLR, i, s \in I_t \tag{3.108}$$

For the clarification technologies, WQ_{tisj} triggers the selection (Eq. (3.109) and Eq. (3.110)).

$$R_{tisc} = \sum_{j \in J_t} rq_{tqcj} \cdot WQ_{tqisj}, \qquad \forall t \in CLR, q \in TCLR, i, s \in I_t, c \in CT_t \tag{3.109}$$

where rq_{tqcj} is the separation efficiency of a clarification technology SED or DAF.

$$\sum_{j \in J_t} WQ_{tqisj} = E_{tis}, \qquad \forall t \in CLR, q \in TCLR, i, s \in I_t \tag{3.110}$$

3.3.3.2 Further linearisations of mass balance constraints

Concentration constraints

Section 3.3.2 demonstrated the reformulation of some of the material balances involved. The bilinear product of the concentrations and removal efficiencies is addressed by substituting Eq. (3.15) with the constraint below:

$$C^F_{tisc} - CR^F_{tisc} - M^{BIG}_c \cdot (1 - E_{tis}) \leq C^P_{tisc} \leq C^F_{tisc} - CR^F_{tisc} + M^{BIG}_c \cdot (1 - E_{tis}), \quad \forall t, i, s \in I_t, c \in CT_t \tag{3.111}$$

where CR^F_{tisc} replaces the aforementioned bilinear product using multiparametric disaggregation technique described previously.

$$CR^F_{tisc} = \sum_{z=lp}^{P} \sum_{k=0}^{9} 10^{lp} \cdot k \cdot \hat{Cr}^F_{tisckz} + \sum_{k=0}^{1} 10^{lp} \cdot k \cdot \bar{Cr}^F_{tisck}, \qquad \forall t, i, s \in I_t, c \quad (3.112)$$

where $\hat{Cr}_{tisckz}$ and $\bar{Cr}_{tisck}$ are a set of continuous non-negative variables the concentrations variable is disaggregated into . The separation efficiency is expressed as a multi-parametric sum of active decimal powers determined by binary variables zr_{tisckz} and continuous variables $\bar{zr}_{tisck}$.

$$R_{tisc} = \sum_{z=lp}^{P} \sum_{k=0}^{9} 10^{lp} \cdot k \cdot zr_{tisckz} + \sum_{k=0}^{1} 10^{lp} \cdot k \cdot \bar{zr}_{tisck}, \qquad \forall t, i, s \in I_t, c \quad (3.113)$$

$$\hat{Cr}^F_{tisckz} \le M^{BIG}_c \cdot zr_{tisckz}, \qquad \forall t, i, s \in I_t, c, k, z \quad (3.114)$$

$$\bar{Cr}^R_{tisck} \le M^{BIG}_c \cdot \bar{zr}_{tisck}, \qquad \forall t, i, s \in I_t, c, k \le 1 \quad (3.115)$$

The connection of $\hat{Cr}_{tisckz}$ and $\bar{Cr}_{tisck}$ with C^F_{tisc} is given in Eq. (3.116) and Eq. (3.117).

$$\sum_{k=0}^{9} \hat{Cr}^F_{tisckz} = C^F_{tisc}, \qquad \forall t, i, s \in I_t, c, z \quad (3.116)$$

$$\sum_{k=0}^{1} \bar{Cr}^F_{tisck} = C^F_{tisc}, \qquad \forall t, i, s \in I_t, c \quad (3.117)$$

$$\sum_{k=0}^{9} zr_{tisckz} = 1, \qquad \forall t, i, s \in I_t, c, z \quad (3.118)$$

Only one significant digit can exist for every technology t, pass i, stage s, contaminant c:

$$\sum_{k=0}^{1} \bar{zr}_{tisck} = 1, \qquad \forall t, i, s \in I_t, c \quad (3.119)$$

The separation efficiency ranges between 0 and 1 and therefore, the power lp is chosen accordingly.

Flowrate constraints

As the recovery for clarification technologies becomes a variable (Eq. (3.120)), the product for the feed flowrate and the recovery has to be linearised.

$$\bar{Y}_{tis} = \sum_{q \in TCLR} (\bar{y}_{qis} \cdot X_{qis}) \qquad \forall t \in CLR, i, s \in I_t \tag{3.120}$$

It is known that the recovery can take either one or another value which does not necessitate a complicated representation such as the multiparametric disaggregation. Therefore, a simple approximation where the recovery is discretised is sufficient.

$$QY^F_{tis} = \sum_r (\bar{Q}^F_{tisr} \cdot \hat{Y}_{tisr}) \qquad \forall t \in CLR,\ i, s \in I_t \tag{3.121}$$

where QY^F_{tis} represents the bilinear product of flowrate and recovery and $\bar{Q}^F_{tisr}$ is an auxiliary continuous variable.

$$\bar{Y}_{tis} = \sum_r (\hat{Y}_{tisr} \cdot zy_{tisr}) \qquad \forall t \in CLR,\ i, s \in I_t \tag{3.122}$$

where zy_{tisr} is a binary variable.

$$\sum_r (zy_{tisr}) = 1 \qquad \forall t \in CLR,\ i, s \in I_t \tag{3.123}$$

$$\bar{Q}^F_{tisr} \leq Q^{IN} \cdot zy_{tisr} \qquad \forall t \in CLR,\ i, s \in I_t \tag{3.124}$$

$$\sum_r (\bar{Q}^F_{tisr} \cdot zy_{tisr}) = Q^F_{tis} \qquad \forall t \in CLR,\ i, s \in I_t \tag{3.125}$$

Thus, the equivalent equations representing the permeate flowrate for CLR are:

$$QY^F_{tis} - Q^{IN} \cdot (1 - E_{tis}) \leq Q^P_{tis} \leq QY^F_{tis} + Q^{IN} \cdot (1 - E_{tis}), \qquad \forall t \in CLR,\ i, s \in I_t \tag{3.126}$$

$$Q^F_{tis} - Q^{IN} \cdot E_{tis} \leq Q^P_{tis} \leq Q^F_{tis}, \qquad \forall t \in CLR,\ i, s \in I_t \tag{3.127}$$

3.3.3.3 Linearisations of operating cost constraints

After having discretised operating conditions, the decision of which level to pick has to be addressed in the ongoing costs which depend on flow, already linearised capacity or production rate, operating conditions and a binary variable. Eq. (3.47) will then alter to Eq. (3.128).

$$CHC_{tis} = cv^{CHC} \cdot t_h \cdot t_d \cdot c^{chem} \cdot QCD_{tis}, \qquad \forall t \in CF, i, s \in I_t \tag{3.128}$$

where QCD_{tis} is the product of flow and selected operating condition when the cost is active. Thus, the additional constraint for the chemical dosage and flowrate is given in Eq. (3.129).

$$QCD_{tis} \leq cd_{tj} \cdot Q^{FL}_{tis} + M^{CD} \cdot (1 - W_{tisj}), \qquad \forall t \in CF, i, s \in I_t, j \in J_t \tag{3.129}$$

where M^{CD} is a big number for the chemical dosage. Minimising the dosage will presumably lead to lower cost, thus, the constraint provided is sufficient. Electrical costs for mixing are modified accordingly in the equation below where QtG_{tis} is the linearised product of flowrate, retention time and energy input.

$$EMC_{tis} = cv^{EM} \cdot t_d \cdot t_h \cdot \mu \cdot c^E \cdot QtG_{tis}, \forall t \in CF, i, s \in I_t \tag{3.130}$$

Two constraints are necessary for representing QtG_{tis} because its resulting cost is a trade-off among the participating variables.

$$QtG_{tis} \leq tf_{tj} \cdot gf^2_{tj} \cdot Q^{FL}_{tis} + M^{TG} \cdot (1 - W_{tisj}), \qquad \forall t \in CF, i, s \in I_t, j \in J_t \tag{3.131}$$

$$QtG_{tis} \geq tf_{tj} \cdot gf^2_{tj} \cdot Q^{FL}_{tis} - M^{TG} \cdot (1 - W_{tisj}), \qquad \forall t \in CF, i, s \in I_t, j \in J_t \tag{3.132}$$

where M^{TG} is a big number for energy input and time. In the saturator and pumping costs, the product of the pressure and flowrate appear (Eq. (3.51) and Eq. (3.52)) which is also substituted by a single continuous variable, QPf_{tis}, shown in Eq. (3.133) and Eq. (3.134).

$$SC_{tis} = \frac{cv^{SC} \cdot c^E \cdot QPf_{tis}}{\eta^{SAT}}, \qquad \forall t \in CLR, i, s \in I_t \tag{3.133}$$

$$PC_{tis} = \frac{cv^{PC} \cdot c^E \cdot QPf_{tis}}{\eta^{FP}_t \cdot \eta^{MT}_t}, \qquad \forall t \notin CLR, i, s \in I_t \tag{3.134}$$

QPf_{tis} is derived from p_{tj}, Q^{FL}_{tis} and W_{tisj} in Eq. (3.135) and Eq. (3.136).

$$QPf_{tis} \leq p_{tj} \cdot Q^{FL}_{tis} + M^P \cdot (1 - W_{tisj}), \qquad \forall t, i, s \in I_t, j \in J_t \tag{3.135}$$

$$QPf_{tis} \geq p_{tj} \cdot Q^{FL}_{tis} - M^P \cdot (1 - W_{tisj}), \qquad \forall t, i, s \in I_t, j \in J_t \tag{3.136}$$

where M^P is a big number for the pressure. It should be pointed out that the pressure values for DAF are the ones CLR adopts. The replacement cost of media for MMF involves only operating characteristics of the filter from which one is singled out in the formulation below.

$$MRC_{tis} = \sum_{j \in J_t} af^{MRC} \cdot rc_t^M \cdot \frac{\pi \cdot l_{tj} \cdot d_{tj}^{MED^2}}{4} \cdot W_{tisj} \qquad \forall t \in MMF, i, s \in I_t \quad (3.137)$$

3.3.3.4 Objective function

The objective function for the MILFP model is to minimise the water net cost, WNC, which equals the total annual cost divided by the annual plant production rate:

$$minimise \quad WNC = \frac{TC}{Q^{AP}}$$

As the objective function is a fraction of two variables, a reformulation is applied for its linearisation. It has been demonstrated that the Dinkelbach's algorithm [Dinkelbach, 1967] finds optimal solution for both, MILFP maximisation and minimisation problems [You et al., 2009, Yue and You, 2013, Liu et al., 2014]. A variation of the algorithm is used in this work to reformulate the objective function and accommodate the MILFP as follows:

$$minimise \quad TC - \alpha \cdot Q^{AP}, \qquad (3.138)$$

where α is a parameter. The objective function is subject to:

- separation efficiencies Eq. (3.107) - Eq. (3.110)
- mass balances Eq. (3.16) - Eq. (3.23),Eq. (3.25) - Eq. (3.30), Eqs. (3.32),Eq. (3.35),Eq. (3.36), Eq. (3.62) - Eq. (3.72), Eq. (3.111) - Eq. (3.127)
- targets Eq. (3.38), Eq. (3.39), Eq. (3.73) - Eq. (3.81)
- logical conditions Eq. (3.40) - Eq. (3.46)
- operating costs Eq. (3.48), Eq. (3.49), Eq. (3.54) - Eq. (3.56), Eq. (3.128) - Eq. (3.137)
- capital costs Eq. (3.84) - Eq. (3.94)
- total annual cost Eq. (3.138)

The algorithm is implemented in two loops whose steps are outlined below and shown in Fig. 3.3.

1. Initialise the parameter α;
2. Relax binary variables related to multi-parametric disaggregation , i.e. zf_{tisckl}, zp_{tisckl}, zc_{tisckl}, zo_{ckl} and zr_{tisckz};
3. Solve the MILP model where the values of the total cost, TC, and the annual production flow, Q^{AP}, returned are designated as TC^* and Q^{AP*};
4. When $\left|TC^* - \alpha \cdot Q^{AP*}\right| \leq \epsilon$, terminate and return the optimal solution $WNC = TC^*/Q^{AP*}$; otherwise update $\alpha = TC^*/Q^{AP*}$ and return to 3;
5. Fix E_{tis} for pass 1 and stage 1 of selected E_{tis} from step 4;
6. Unrelax zf_{tisckl}, zp_{tisckl}, zc_{tisckl}, zo_{ckl} and zr_{tisckz};
7. Solve the MILP model where the values of the total cost, TC, and the annual production flow, Q^{AP}, returned are designated as TC^* and Q^{AP*};
8. When $\left|TC^* - \alpha \cdot Q^{AP*}\right| \leq \epsilon$, terminate and return the optimal solution $WNC = TC^*/Q^{AP*}$; otherwise update $\alpha = TC^*/Q^{AP*}$ and return to 7.

The approximations and linearisations contribute to the heavy size of the model and therefore, increase in the computational performance. Therefore, Dinkelbach's algorithm has been applied two consecutive times, once with relaxed binary variables derived from reformulations and a second time when the binary variables are not relaxed. It has been deducted this strategy reduces the computational time immensely.

3.3.4 Models summary

The objective functions and constraints valid for models $P0$, $P1$ and $P2$ are summarised and listed in Table 3.3.

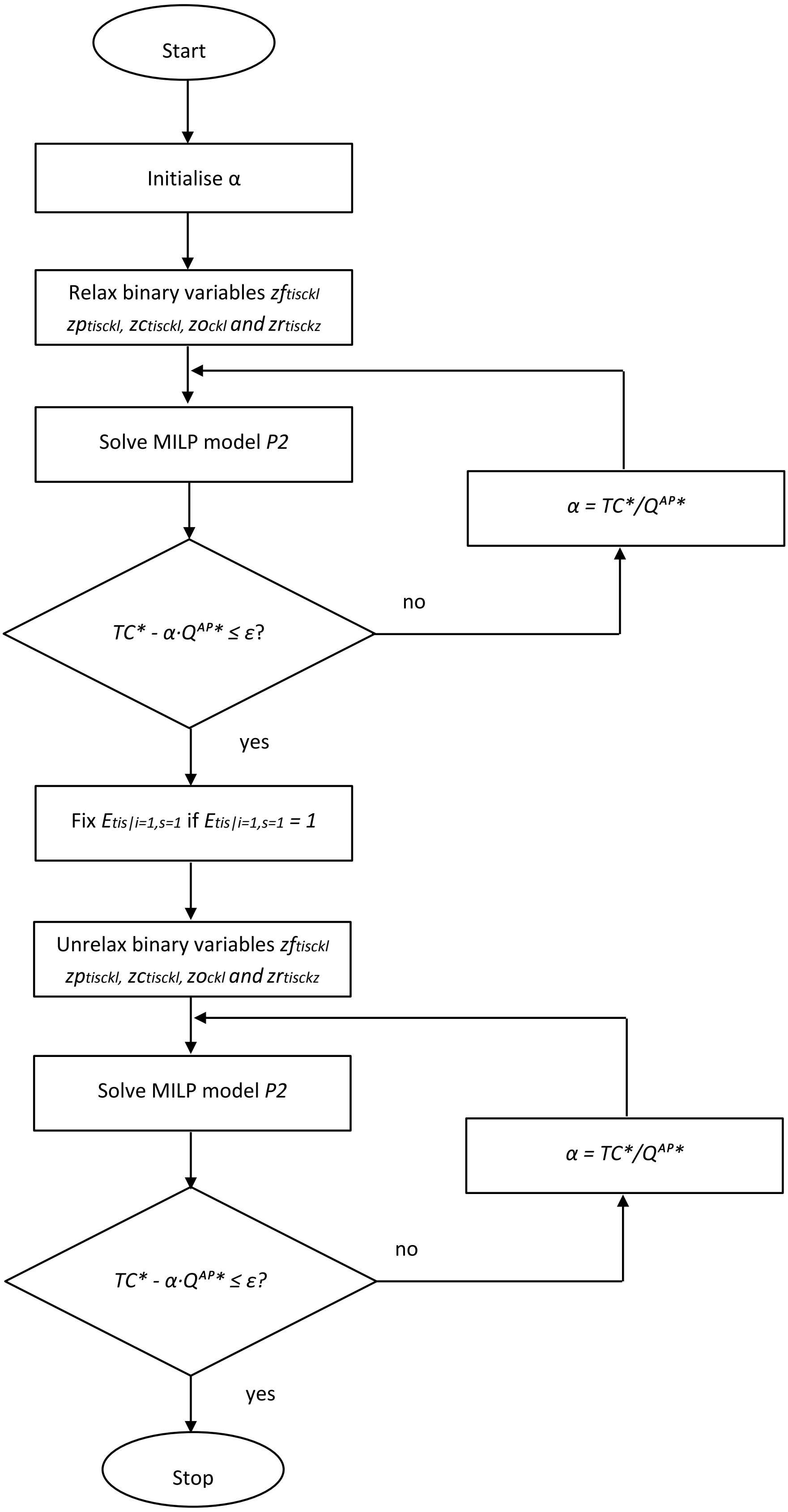


Figure 3.3: Algorithm for solving MILFP model $P2$

Table 3.3: Summary of constraints and objective functions for MINLP, plMINLP and MILFP models

Constraints	MINLP model ($P0$)	plMINLP model ($P1$)	MILFP model ($P2$)
separation efficiencies	Eq. (3.2) - Eq. (3.14)	Eq. (3.2) - Eq. (3.14)	Eq. (3.107) - Eq. (3.110)
mass flow balance	Eq. (3.15) - Eq. (3.36)	Eq. (3.15) - Eq. (3.30), Eqs. (3.32), Eq. (3.35), Eq. (3.36), Eq. (3.62) - Eq. (3.72)	Eq. (3.16) - Eq. (3.23),Eq. (3.25) - Eq. (3.30), Eq. (3.35),Eq. (3.36), Eq. (3.62) - Eq. (3.72), Eq. (3.111) - Eq. (3.127)
target purity	Eq. (3.37) - Eq. (3.39)	Eq. 3.38, Eq. (3.39), Eq. (3.73) - Eq. (3.81)	Eq. (3.38), Eq. (3.39), Eq. (3.73) - Eq. (3.81)
logical conditions	Eq. (3.40) - Eq. (3.46)	Eq. (3.40) - Eq. (3.46)	Eq. (3.40) - Eq. (3.46)
operating costs	Eq. (3.47) - Eq. (3.56)	Eq. (3.47) - Eq. (3.56)	Eq. (3.48), Eq. (3.49), Eq. (3.54) - Eq. (3.56), Eq. (3.128) - Eq. (3.137)
capital costs	Eq. (3.57) - Eq. (3.58)	Eq. (3.84) - Eq. (3.94)	Eq. (3.84) - Eq. (3.94)
total annual cost	Eq. (3.60)	Eq. (3.60)	Eq. (3.60)
objective function	Eq. (4.61)	Eq. (4.61)	Eq. (3.138)

Unlike in models $P0$ and $P1$, in model $P2$, a hierarchical solution approach is applied by solving the Dinkelbach's algorithm twice in a sequential manner - once with relaxed binary variables which appear in the multiparametric disaggregation technique. The results from both, $P1$ and $P2$ are post-processed with $P0$ immediately after $P1$ and $P2$ in order to (i) obtain exact and not approximated solution and (ii) be able to compare the solutions with the ones obtained from $P0$. Scaling the variables and equations for the models has been performed accordingly.

3.4 Illustrative examples

To illustrate the capability of the four proposed approaches, they have been applied to two theoretical examples with data from industrial practices. The first case study looks at seawater desalination while the latter examines surface water treatment; both to produce drinking water.

3.4.1 Seawater desalination example

Countries with arid land and prolonged droughts have included in their water supply planning sources such as seawater. Consequently, a number of seawater desalination projects have already been realised and many are contracted to be completed in the near future. With an outlook of the foreseen trends, the first example focuses its attention on seawater desalination plants design. Thus:

- **Intake and production capacities**. The water intake $Q^{IN} = 55,000\, m^3/h$ for a system with minimum allowable effluent $M^{FLOW} = 5,000\, m^3/h$ which, for instance, corresponds to the production capacity of Carboneras SWRO plant in Spain. Additional production capacities of membrane desalination plants not only in Spain but in Algeria, US, China and India predominantly vary between $4,000\, m^3/h$ and $10,000\, m^3/h$ [Abengoa Water, 2016]. One of the largest membrane seawater desalination projects is situated in Ras Alkhair (Saudi Arabia) where it provides circa $41,667\, m^3/h$ [Better World Solutions, 2016]. Seawater intakes, on the other hand, must be more than twice as much as the desired production rate in order to overcome the low yield of the membrane plants. For example, Adelaide

Desalination Plant's (Australia) intake capacity approximates $28,400\,m^3/h$ with production capacity of roughly $12,500\,m^3/h$ and Qingdao Desalination Plant's (China) intake capacity surpasses $10,000\,m^3/h$ with an output of $4,167\,m^3/h$ [Acciona Agua, 2016, Clemente, 2013].

- **Intake and product quality**. The quality of the seawater ranges from $30,000\,mg/L$ to $40,000\,mg/L$ TDS depending on the location of the sea or ocean [American Water Works Association, 2007]. The TSS and boron have typical values of $30\,mg/L$ and $5\,mg/L$, respectively [Tchobanoglous et al., 2003, Mane et al., 2009], which are the values used for the initial concentrations of contaminants in the source water. The final contaminants concentrations for drinking water must not exceed $600\,mg/L$, $1\,mg/L$ and $2.4\,mg/L$ for TDS, TSS and boron according to regulatory standards [The Drinking Water Inspectorate, 2009, U.S. Environmental Protection Agency, 2010, World Health Organization, 2011].

- **Performance parameters**. Conventional technologies using chemicals exhibit a removal mechanism where it can be assumed that essentially they operate at almost full recovery. Hence, CF, SED and DAF's recoveries are set at 99 %. The recoveries of the filters can reach 100 %, however, it is more likely they lie between 85% and 95% [US Interior Reclamation Department, 2013], therefore, a value of 95 % is used. The high pressure membranes manifest lower percentage recoveries and based on reported values in literature [Lu et al., 2006, Mickley et al., 2006], 80 % is effective for NF and 45 % for RO. A satisfactorily performing coagulant in seawater and hence, often the choice is ferric coagulant which costs roughly $\$\,250/tonne$. The dosage range used in the model is $1mg/L$-$20mg/L$. The labour cost coefficients $lc1 = 148.9$ and $lc2 = 69,289$ are derived from a set of data from Contra Costa Water District et al. [2007]. In the same source, chemical costs involved in filtration, desalination and post-treatment as a function of the filtered product have been reported which have been aggregated in the current work to $r^{ch} = 0.0326\$/m^3$. The costs have been converted to SI units and the inflation has been accounted for. Additional performance and costing parameters for models can be found in Table 3.4 and the remaining of the data are reported elsewhere [Koleva et al., 2016a]. It must be noted that in Table 3.4, the replacement cost, rc_t^M, for MMF and the membrane technologies differs significantly as the former is the cost per cubic metres media while the latter is the cost per filtrate produced. The discretised data for model $P2$ is located in the Supplementary Material.

- **Passes and stages**. Considering that the recovery of the CF and CLR is practically complete, and furthermore, following the pattern of industrial practices where vessels are attached in series only, in this work, the number of passes (chambers in series) equals to 3 and the number of stages - to 1. Filters, in particular membrane systems can take up configurations of various numbers of passes and stages where London's Desalination Plant, for example, has a 4-pass, 4-stage RO system. In this example, we allow 3 passes and 3 stages for every filtration technology.

3.4.2 Surface water treatment example

Despite disruptive climatic changes and aquifer depletion, drinking water treatment plants (DWTP) with surface water intake are the main and socially accepted method for obtaining potable water. Consequently, the pick for the second case study in the current chapter.

- **Intake and production capacities**. The water intake $Q^{IN} = 10,000\,m^3/h$ for a system with minimum allowable effluent $M^{FLOW} = 2,000\,m^3/h$ which, for instance, falls in the middle of the production capacities of the DWTPs in Dogubayazit, Turkey ($1,458.3\,m^3/h$) and El Conquero, Spain ($3,750\,m^3/h$). Drinking water treatment plants generally exhibit a higher yield with maximum abstraction twice as much as the production capacity. At Ballyfarnan DWTP for instance, the intake is $135\,m^3/h$ whereas the production rate capacity is estimated as $75\,m^3/h$. Similarly, Rockingham DWTP abstracts $500\,m^3/h$ at most to produce maximum $250\,m^3/h$ [Doris, 2015, Doris et al., 2015]. At the world's largest Water Purification Plant in Chicago, Illinois - the James W. Jardine $41,666,666\,m^3/h$ are treated on average [Center for Mechanical Simulation Technology, 2011]. Typical DWTP sizes enclose production capacities from $1,000\,m^3/h$ to $15,000\,m^3/h$ [Abengoa Water, 2016].

- **Intake and product quality**. Unlike in seawater, boron is not present in abundance. In surface water, however, the organic content of the water is taken into account. Hence, the quality of the source water is: $200\,mg/L$ TSS, $800\,mg/L$ TDS and 30 mg/L COD [Tchobanoglous et al., 2003, Cheremisinoff, 2002, Chowdhury et al., 2013]. The final contaminants concentrations for drinking water must not exceed 600 mg/L, 1 mg/L and 5 mg/L for TDS, TSS and COD according to regulatory standards [The Drinking Water Inspectorate, 2009, U.S. Environmental Protection Agency, 2010, World Health Organization, 2011].

- **Performance parameters**. In surface water treatment, the preferred choice for coagulant is aluminium sulphate (alum) due to its cheaper price of approximately \$ 150/*tonne* [Global B2B Marketplace, 2015]. Its dosage also differs by increasing to 10mg/L - 30mg/L. CF cannot take a full recovery because of its separating performance for COD. Thus, a value of 0.99 is assumed. Additionally, viscosity value of 1.000 $kg/m \cdot s$ at ambient temperature is taken. Reverse osmosis has a higher recovery (see Table 3.5) due to the lower salt content in the water. The rest of the data overlaps with the given data from Section 3.4.1.

- **Passes and stages**. The same number of allowed passes and stages is adopted from the example in Section 3.4.1.

Table 3.4: Seawater desalination: pressure design variables, efficiencies and economic parameters

Technology	CF	CLR SED / DAF	MMF	MF	UF	NF	RO1	RO2
y_{tis} range $[-]$	1	0.99/0.99	0.95	0.95	0.95	0.80	0.45	0.45
P_{tis} range $[MPa]$	0.1 - 0.2	- / 0.4 - 0.7	0.1 - 0.2	0.1 - 0.2	0.1 - 0.3	0.5 - 1.6	5.0 - 6.0	5.0 - 6.0
η_t^{FP} $[-]$	0.75	- / 0.75	0.80	0.80	0.75	0.80	0.75	0.75
η_t^{MT} $[-]$	0.95	- / 0.95	0.93	0.95	0.97	0.95	0.98	0.98
rc_t^M $[\$/m^3]$	-	- / -	12,359	0.00396	0.00396	0.0528	0.0528	0.0528
$infl_t$ $[-]$	1.143	1.288/1.087	1.319	1.087	1.087	1.511	1.511	1.511
A_t $[-]$	121,701	8,334 / 4,167	69,547	45,601	45,601	158,177	158,177	158,177
$b_t[-]$	0.6	0.6 / 0.6	0.6	0.6	0.6	0.6	0.6	0.6

Source: Lu et al. [2006], Bastaki [2004], Hassan et al. [1999], Adham et al. [2006], European Commission [2003], Wang et al. [2010], Whitman et al. [2002], University of New Hampshire [2016], Mallevialle et al. [1996], Contra Costa Water District et al. [2007], FilterWater [2016], US Inflation Calculator [2016]

Table 3.5: Surface water treatment: pressure design variables, efficiencies and economic parameters

Technology	CF	CLR SED / DAF	MMF	MF	UF	NF	RO1	RO2
y_{tis} range $[-]$	0.99	0.99/ 0.99	0.95	0.95	0.95	0.80	0.6	0.6
P_{tis} range $[MPa]$	0.1 - 0.2	- / 0.4 - 0.7	0.1 - 0.2	0.1 - 0.2	0.1 - 0.3	0.5 - 1.6	3.0 - 5.0	3.0 - 5.0
η_t^{FP} $[-]$	0.75	- / 0.75	0.80	0.80	0.75	0.80	0.75	0.75
η_t^{MT} $[-]$	0.95	- / 0.95	0.93	0.95	0.97	0.95	0.98	0.98
rc_t^M $[-]$	-	- / -	12,359	0.00396	0.00396	0.0132	0.0132	0.0132
$infl_t$ $[-]$	1.143	1.288/1.087	1.319	1.087	1.087	1.511	1.511	1.511
A_t $[-]$	121,701	8,334 / 4,167	69,547	45,601	45,601	158,177	158,177	158,177
$b_t[-]$	0.6	0.6 / 0.6	0.6	0.6	0.6	0.6	0.6	0.6

Source: Lu et al. [2006], Bastaki [2004], Hassan et al. [1999], Adham et al. [2006], European Commission [2003], Wang et al. [2010], Whitman et al. [2002], University of New Hampshire [2016], Mallevialle et al. [1996], US Inflation Calculator [2016], Contra Costa Water District et al. [2007], FilterWater [2016], Nunes and Peinemann [2006]

Multiparametric disaggregation with $p = \{2, 3, 4\}$ for concentrations and flowrates, and with $lp = \{-3, -2, -1, 0\}$ for concentrations and separation efficiencies have lead to reaching optimality gaps 0% for $P1$ and $P2$ and no further refinement was necessary. The conclusion applied to both case studies.

3.5 Computational results and discussion

The developed MINLP and plMINLP models have been tested on various solvers while the MILFP model has been implemented using CPLEX 12.6.3 in GAMS 24.7.1 on a PC with Intel Core $i7-3770$ CPU $3.40\,GHz$, RAM $16\,GB$. The relative optimal gap has been set to 0% for models $P0$ and $P1$. A 90 % gap has been used for each MILP model, in both loops of the Dinkelbach algorithm, which does not compromise the optimality of the final solution, unless larger than 100 % gap is used [Liu et al., 2014]. The reason is that during the last iteration of the algorithm, the objective function is very close to zero, while the upper bound is always positive and the lower bound - always negative. The difference between the two will always be larger than 100% until the epsilon condition is fulfilled.

3.5.1 Seawater desalination results

First, the performance of the proposed models with respect to their computational statistics and objective function is investigated. Then, the flowsheet configurations, and cost breakdown analysis and comparison are performed relative to each model and common industrial practices.

3.5.1.1 Computational statistics

Several deterministic non-linear solvers have been used for models $P0$ (MINLP) and $P1$ (plMINLP). A time limit of $10,000\,s$ has been set for all of them. As shown in Table 3.6, ANTIGONE demonstrates overall better results with significantly lower CPU times than BARON. Although BARON finds the best optimal solution for the MINLP model, its solution deteriorates for the plMINLP model. The former solution is found at CPU time $632\,s$ corresponding to a 0.004 % gap which did not improve by the end of the resource limit time. However, a complete convergence does not occur within the assigned resource limit. The plMINLP model terminates at a gap of 50 % and an objective function of US\$1.0588/m^3 is returned. SCIP, DICOPT and SBB do not provide any solution for any of the two models. The post-processing of the results is a necessary step to obtain a corrected result of the linearisations and approximations made in $P1$ and $P2$. For the plMINLP model, post-processing is performed with the same solver that is implemented in the optimisation runs, whereas for the MILFP model, ANTIGONE was used.

Table 3.6: Computational statistics and comparative results of seawater desalination example

	MINLP model (P0)	**plMINLP model (P1)**	**MILFP model (P2)**
Discrete variables	96	18,780	27,243
Continuous variables	1,237	23,239	31,295
Equations	1,673	28,217	39,992
Solvers	Objective function [US\$/m^3]	(CPU time)	
Antigone	0.8363 (120s)	0.7346* (1,499s)	-
Baron	0.7346 (10,000s)	1.0588* (10,000s)	-
Cplex	-	-	0.7346* (388s)

* after post-processing results with MINLP

The models statistics of the seawater desalination case study are also given in Table 3.6. It can further be concluded from the table that all the implemented reformulations in $P2$ have lead to almost 24 times larger model size than $P0$. Although the number of equations and variables increase with the models, it can be observed the solution improves with ANTIGONE. Compared to $P1$, $P0$ returns results one order of magnitude as fast, at the expense of a worse solution. The post-processed results for $P1$ and $P2$ prove a better solution exists which is 11% better than the solution in $P0$. Furthermore, the implemented approximations have translated in a tight difference, i.e. 0.4% from the real solutions. From the table it becomes ostensible that model $P2$ has the upper hand in the trade-off between computational times and objective function, with respect to the rest of the models. The reported solution for MILFP at optimal gap 90% translated to 3 iterations for the first loop and 4 iterations for the second one.

The flowsheet configurations and cost comparisons in the following sections are presented based on the solutions reported by ANTIGONE of $P0$ and $P1$, and the post-processed results of $P1$ and $P2$. Post-processing of the results involved fixing the optimal flowsheet obtained from the linearised models and solving the original $P0$ model, which resulted in the reported values in Table 3.6. This is a proof that the solution obtained from $P2$ is a real solution and its computational performance is superior to model $P0$ and $P1$.

3.5.1.2 Flowsheet configurations

The flowsheet configurations for the proposed models are depicted in Fig. 3.4 and Fig. 3.5. The conceptual design for the MINLP model contains one CF, three DAF chambers in series, two passes MMF, two passes NF and one-pass, two-stage RO system. The choice for conventional technologies in pre-treatment with a sequence of coagulation-flocculation and dissolved air flotation is one of the typical possible combinations in practice. Globally, DAF and UF have an installed capacity of 19 % while MMF's installed capacity accounts for 49% [DesalData, 2014]. The second stage in the reverse osmosis configuration contributes to the higher overall recovery of the flowsheet, i.e. 39 %, which is slightly lower than in existing desalination plants. The total number of units is 10, which is the maximum allowed number of units, i.e. the constraint is active. The final purity of the product is 1.000 mg/L TSS, 600 mg/L TDS and 0.799 mg/L boron thus, meeting drinking water requirements. The full concentrations and flowrates profiles of the flowsheet in Fig. 3.4 are shown in Table 3.7.

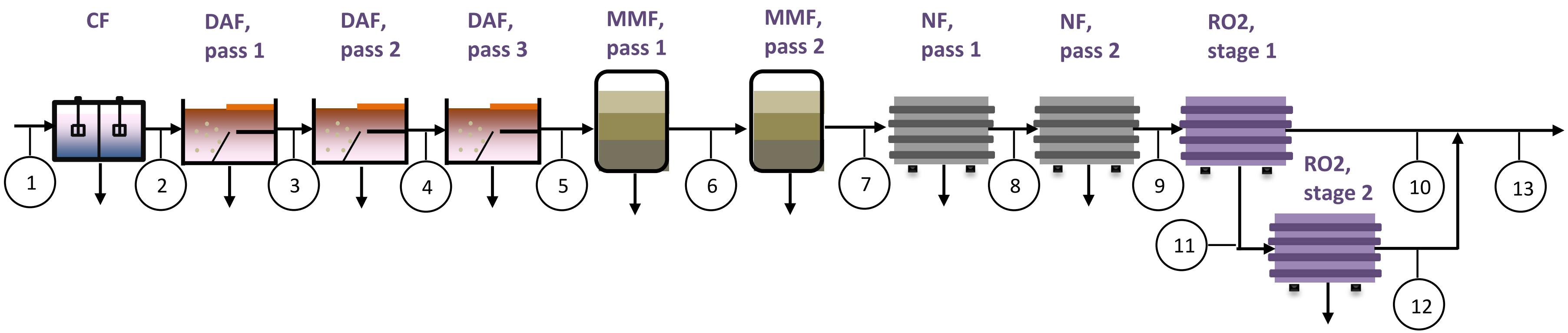


FIGURE 3.4: Optimal flowsheet configuration for $P0$ model for seawater desalination case study

Table 3.7: Concentration and flowrate profiles for $P0$ model for seawater desalination case study

Stream	Concentrations			Flowrates
	TSS $[mg/L]$	TDS $[g/L]$	B $[mg/L]$	$[m^3/h]$
1	30.00	40.00	5.00	55,000
2	30.00	40.00	5.00	55,000
3	21.21	40.40	5.05	54,450
4	12.34	40.81	5.10	53,906
5	3.37	41.22	5.15	53,366
6	1.14	43.39	5.42	50,698
7	0.45	45.68	5.71	48,163
8	0.56	4.12	7.14	38,531
9	0.69	0.42	8.92	30,824
10	1.55	0.93	0.78	13,871
11	-	-	15.58	16,953
12	-	-	0.83	7,629
13	1.00	0.60	0.79	21,500

Since the same objective function was observed for $P1$ and $P2$, their technology selection is also the same, hence, presented in a common figure. In Fig. 3.5, the flowsheet consists of three UF passes, two NF passes and one - pass, three - stage RO system. Although, solely 1 % of desalination worldwide is performed by NF, it has been gaining more interest recently due to lower operating costs and higher yield [DesalData, 2014]. Therefore, the flowsheet has kept the selection of TDS removal system from $P0$. The selection of a three - stage configuration for the RO system has been a preferred choice in order to increase the productivity of the plant and therefore, decrease the cost. With this configuration, the plant is capable of producing $25,158\,m^3/h$, i.e. circa 46% total recovery, which means 7 % improvement compared to the recovery for the flowsheet in Fig. 3.4. The water quality of the effluent is $0.40 mg/L$ TSS, $600 mg/L$ TDS and $0.29 mg/L$ boron for $P1$ and $0.40 mg/L$ TSS, $600 mg/L$ TDS and $0.61 mg/L$ boron for $P2$. The discrepancy in the boron concentrations come from the different pH selected for stage 2 of the reverse osmosis. The pH is not reflected in the operating cost therefore, it affects only the rejection. In Table 3.8 all the concentrations and flowrates of flowsheet in Fig. 3.5 are listed.

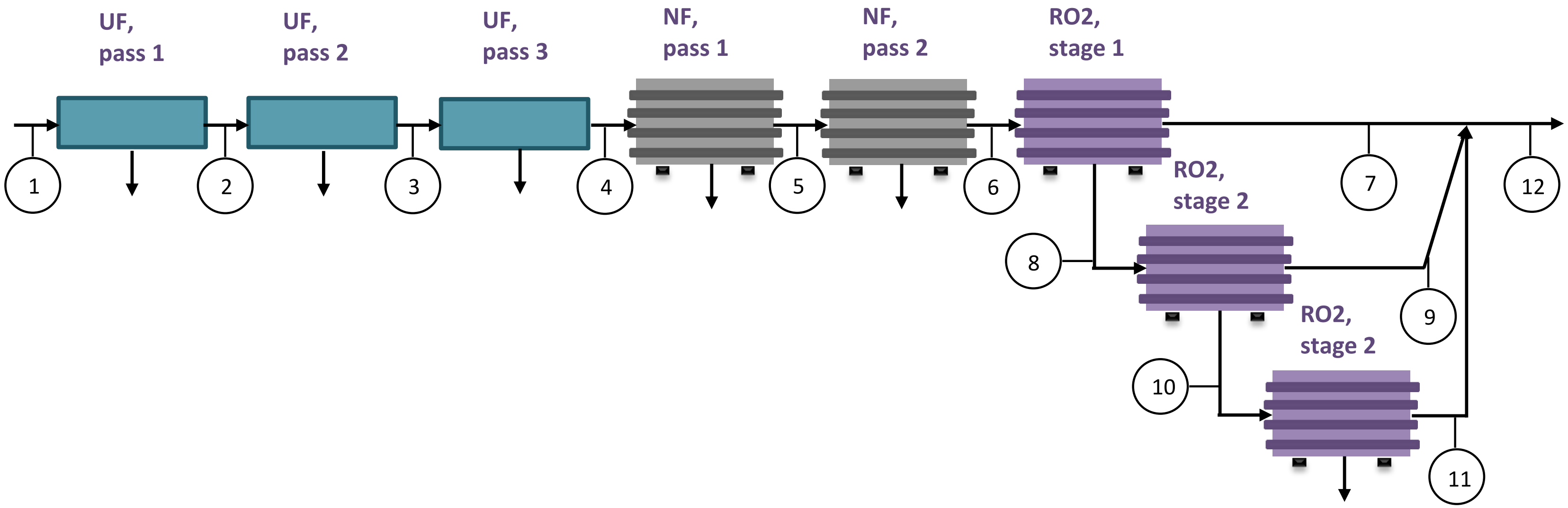


FIGURE 3.5: Optimal flowsheet configuration for $P1$ and $P2$ models for seawater desalination case study

TABLE 3.8: Concentration and flowrate profiles for $P1$ and $P2$ models for seawater desalination case study

Stream	plMINLP model				MILFP model			
	Concentrations			Flowrates	Concentrations			Flowrates
	TSS $[mg/L]$	TDS $[g/L]$	B $[mg/L]$	$[m^3/h]$	TSS $[mg/L]$	TDS $[g/L]$	B $[mg/L]$	$[m^3/h]$
1	30.00	40.00	5.00	55,000	30.00	40.00	5.00	55,000
2	5.76	42.07	5.26	52,250	5.76	42.07	5.26	52,250
3	1.11	44.27	5.54	49,638	1.11	44.27	5.54	49,638
4	0.21	46.65	5.83	47,156	0.21	46.65	5.83	47,156
5	0.27	4.20	7.28	37,725	0.27	4.20	7.28	37,725
6	0.33	0.50	9.11	30,180	0.33	0.50	9.11	30,180
7	0.74	1.12	0.18	13,580	0.74	1.11	0.18	13,580
8	-	-	16.42	16,599	-	-	16.42	16,599
9	-	-	0.32	7,470	-	-	1.44	7,470
10	-	-	29.68	9,129	-	-	28.68	9,129
11	-	-	0.57	4,108	-	-	0.55	4,108
12	0.40	0.60	0.29	25,158	0.40	0.60	0.61	25,158

3.5.1.3 Costing comparisons

The cost breakdown differences in the MINLP model, and the plMINLP and MILFP models are disclosed in Fig. 3.6 where every cost component is represented as a percentage of the cost per water volume produced. Included in the cost breakdown are the annual labour, power, capital, replacement, chemical for treatment and conditioning, and post-treatment chemical costs. The lower number of units in models $P1$ and $P2$ contribute to capital cost representing 30 % of the total cost compared to a capital cost share of 35 % for $P0$. Typical ranges of capital costs are between 30 % and 40 % of the total cost for seawater desalination facilities. The elevated percentage of power cost for $P1$ and $P2$ with respect to $P0$ is due to the higher number of RO units selected, which overall contribute to a lower water net cost. Approximately 13 % of running costs is for maintenance and consumables which is also observed for all of the presented models and is comparable to the lower range of operating and maintenance costs in existing practices [Voutchkov, 2013].

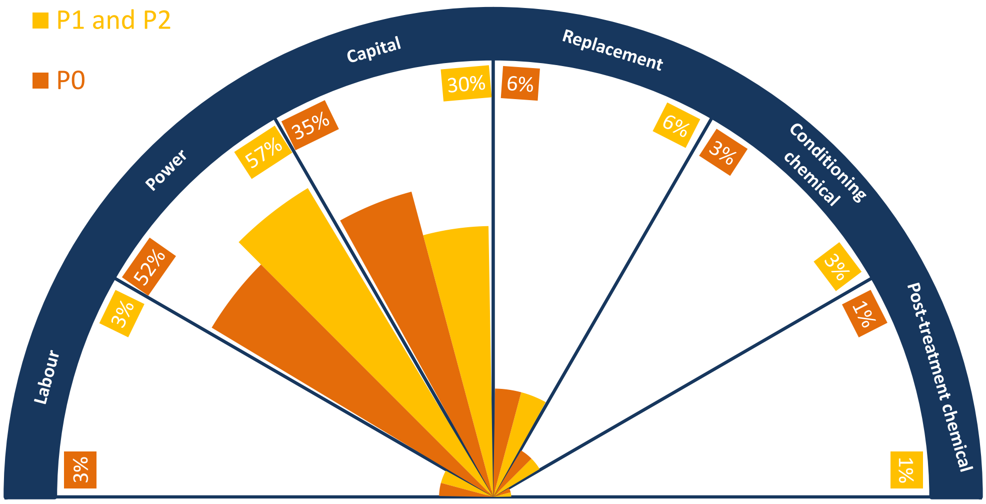


FIGURE 3.6: Cost breakdown comparison among proposed models for seawater desalination case study

3.5.1.4 Comparisons with existing plants

According to the International Water Association (IWA), seawater desalination water net cost lies between US$0.5/$m^3$ and US$3.0/$m^3$ [Lazarova et al., 2012]. Furthermore, this range coincides with the range reported by Voutchkov [2013]. The optimal solution returned by ANTIGONE and CPLEX was US\$0.7346/m^3 and consequently, the result fell into the suggested limits. Kurnell and Victorian desalination plants in New South Wales and Victoria, for instance, produce at maximum $500,000\,m^3/d$ and $550,000\,m^3/d$ at respective costs US\$1.75/m^3 and US\$1.78/m^3 [UNESCO Centre for Membrane Science and Technology, 2008]. In comparison, the production rate of the best optimal solution obtained from plMINLP and MINLP models is around $600,000 m^3/d$ with 60 % lower cost.

3.5.2 Surface water treatment results

3.5.2.1 Computational statistics

The models statistics and comparative results of the surface water treatment case study are shown in Table 3.9.

TABLE 3.9: Computational statistics and comparative results of surface water treatment example

	MINLP model (P0)	**plMINLP model (P1)**	**MILFP model (P2)**
Discrete variables	87	16,305	23,568
Continuous variables	1,117	20,230	26,640
Equations	1,652	24,695	34,790
Solvers	Objective function [US\$/m^3]	(CPU time)	
Antigone	0.5346 (160s)	0.1888* (466s)	-
Baron	No solution (10,000s)	0.1888* (3,946s)	-
Cplex	-	-	0.1888* (138s)

* after post-processing results with MINLP

Unlike ANTIGONE, BARON fails to return a solution for $P0$. It can be observed, however, both ANTIGONE and BARON perform equally well and obtain the same results for $P1$. Yet, ANTIGONE outperforms BARON with CPU times 90 % lower. SCIP, DICOPT and SBB do not provide any solution for any of the two models.

Models $P1$ and $P2$ returned the same solution of US\$0.1870/m^3 which has been corrected by post-processing those results to US\$0.1888/m^3, meaning only approximately 0.5% has been the underestimation in the objective function. On the other hand, the improvement from the MINLP model is more than twofold. The best trade-off between CPU times and obtained solution is seen in the MILFP model which is an order of magnitude faster than model $P1$. The reported solution for MILFP at optimal gap 90% translated to 4 iterations in the first loop and 3 iterations in the second loop. Overall, the results from the surface water treatment case study follow the same trends as the results from seawater desalination case study.

The flowsheet configurations and cost comparisons are presented based on the solutions reported by ANTIGONE of $P0$ and $P1$, and the post-processed results of $P1$ and $P2$.

3.5.2.2 Flowsheet configurations

The locally optimal solution for $P0$ translates into a technology configuration (Fig. 3.7) of two CF chambers in series, one pass MMF, three MF passes, two UF passes and a one-pass, two-stage RO system. The design is capable of an hourly production rate of $12,104\, m^3/h$. The final concentrations of COD, TSS and TDS are, respectively, $4.08\, mg/L$, $1.00\, mg/L$ and $275\, mg/L$ thus, meeting drinking water requirements. Additionally, the maximum allowable number of technologies is reached. In practice, drinking water treatment plants have less complicated flowsheet design than the one illustrated in the figure. Table 3.10 displays the concentrations and flowrates profiles of the flowsheet in Fig. 3.7.

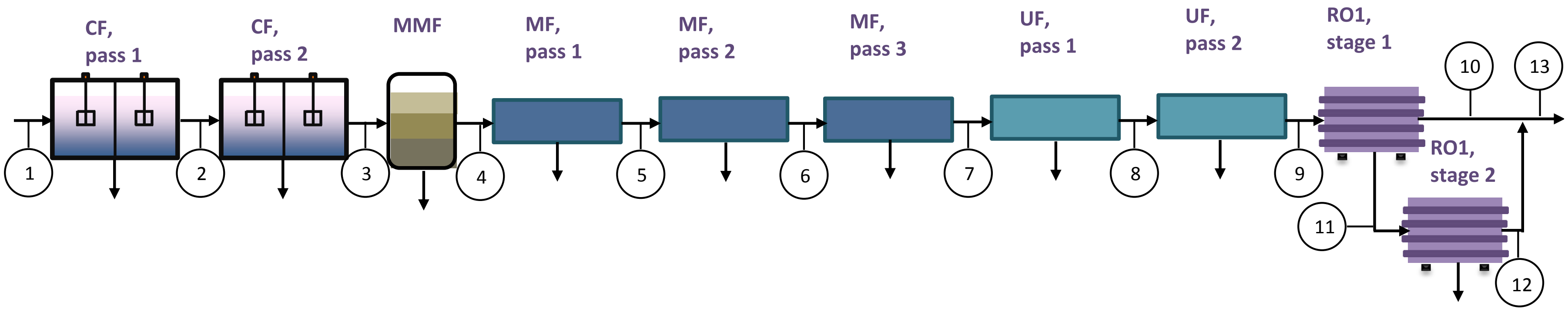


FIGURE 3.7: Optimal flowsheet configuration for $P0$ model for surface water treatment case study

TABLE 3.10: Concentration and flowrate profiles for $P0$ model for surface water treatment case study

Stream	Concentrations			Flowrates
	COD $[mg/L]$	TSS $[mg/L]$	TDS $[g/L]$	$[m^3/h]$
1	30.00	100.00	4.00	20,000
2	21.21	99.99	4.04	19,800
3	12.34	99.99	4.08	19,602
4	12.98	52.98	4.30	18,622
5	9.21	39.92	4.52	17,691
6	6.54	30.16	4.76	16,806
7	4.65	22.79	5.01	15,966
8	3.99	4.38	5.27	15,168
9	3.43	0.84	5.55	14,409
10	5.72	1.40	0.19	8,646
11	-	-	13.59	5,764
12	-	-	0.48	3,458
13	4.08	1.00	0.27	12,104

The flowsheet configuration of $P1$ and $P2$, like in the seawater desalination case study, is the same and shown in Fig. 3.8. The sequence of technologies is with three UF passes and one NF pass. This flowsheet is capable of producing $13,71\,m^3/h$ and potable water with COD, TSS and TDS specifications $4.05\,mg/L$, $0.885\,mg/L$ and $600\,mg/L$ for $P1$ and $5.0\,mg/L$, $0.885\,mg/L$ and $600\,mg/L$ for $P2$ (see Table 3.11). The discrepancy in the COD concentrations arises from the different values for molecular weight cut-off of nanofiltration, in $P1$ $MWCO = 300\,Da$ and in $P2$ $MWCO = 372\,Da$. Molecular weight cut-off, like pH, is also not expressed in the operating costs, hence, differences are plausible.

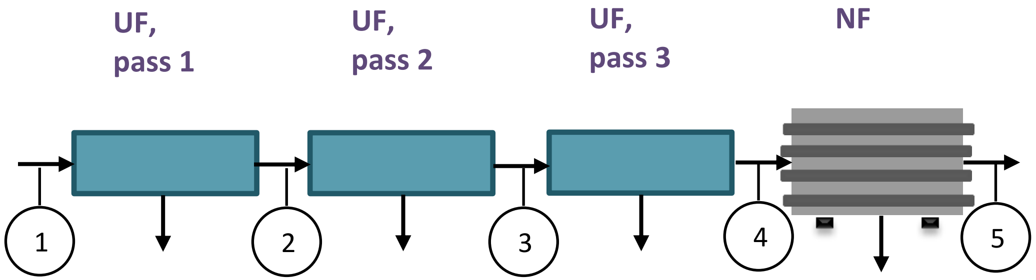


FIGURE 3.8: Optimal flowsheet configuration for $P1$ and $P2$ models for surface water treatment case study

TABLE 3.11: Concentration and flowrate profiles for $P1$ and $P2$ models for surface water treatment case study

Stream	plMINLP model				MILFP model			
	Concentrations			Flowrates	Concentrations			Flowrates
	COD $[mg/L]$	TSS $[mg/L]$	TDS $[g/L]$	$[m^3/h]$	COD $[mg/L]$	TSS $[mg/L]$	TDS $[g/L]$	$[m^3/h]$
1	30.00	100.00	4.00	20,000	30.00	100.00	4.00	20,000
2	25.78	19.20	4.21	19,000	25.78	19.20	4.21	19,000
3	22.15	3.69	4.43	18,050	22.15	3.69	4.43	18,050
4	19.04	0.71	4.67	17,148	19.04	0.71	4.67	17,148
5	4.05	0.89	0.60	13,718	5.00	0.89	0.60	13,718

3.5.2.3 Costing comparisons

The costs breakdown and comparisons for $P0$, and $P1$ and $P2$ are manifested in Fig. 3.9. Unlike for seawater desalination, surface water treatment capital costs in general take a more considerable fraction from the total costs. Opposed to capital costs, the power expenses percentage is lower. The commonly involved lower and upper percentages for power costs in industry are 10 % and 22 % and it can be deducted both of the values in the figure fall in the interval. Mixing and pumping account for 37 % in $P0$ and pumping represents 16% of the total cost in $P1$ and $P2$, which falls in the reported range. In practice, low salinity plants exhibit capital cost fraction between 0.4 and 0.6 [Voutchkov, 2013]. All of the models have a capital cost percentage in the middle of the range. Ongoing costs to total cost ratio is higher (8 % - 22 %) in water treatment plants due to the chemicals usage for removal of COD and TSS. The increase of conditioning chemical from $P0$ to $P1$ and $P2$ can be explained with the lower unit number and higher effluent, therefore, greater amount of chemicals used.

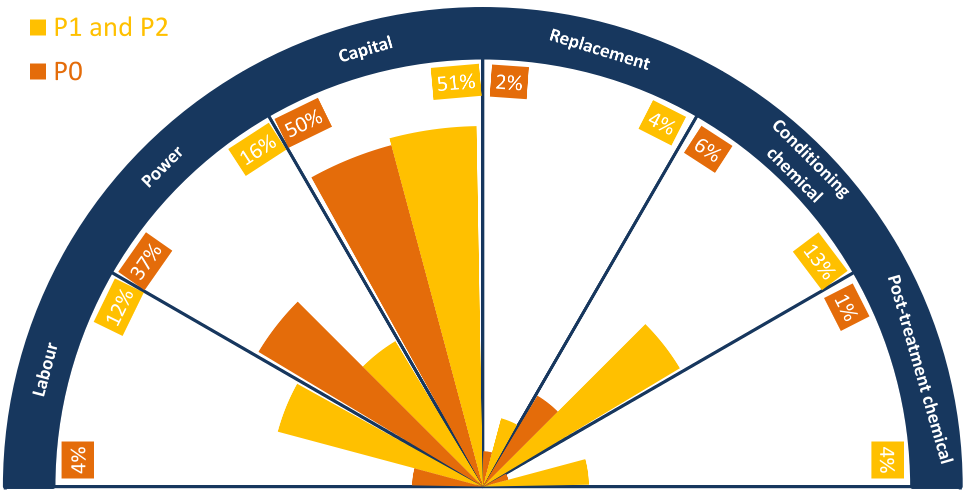


FIGURE 3.9: Cost breakdown comparison among proposed models for surface water treatment case study

3.5.2.4 Comparisons with existing plants

The production cost of drinking water from surface water is situated at the lower end of brackish water treatment processes costs. Ben Aim [2013] reported costs between US\$0.2/m^3 and US\$0.3/m^3 whereas Voutchkov [2013] gave a range of US\$0.2/m^3 -

US\$0.4/m^3. For the minimisation problem we are considering, the water net cost of the improved formulations is $US\$0.188/m^3$. The results are in proximity of the lower end of the reported ranges and thus, show conformity with existing practices.

3.6 Concluding remarks

In this chapter, optimisation-based frameworks for the synthesis of water treatment processes have been proposed. First, the MINLP model has been extended to incorporate alternative purification paths with the objective to minimise water net cost. The large number of non-linearities have compromised the stability of the model by using various commercial MINLP solvers, which either obtained local optimum or even failed to return a feasible solution. To overcome the difficulties, key bilinear terms and non-linear functions have then been reformulated, and the plMINLP model has been introduced. Finally, the MILFP model has been proposed, which includes further discretisations of continuous domains together with a two-step iterative solution procedure based on Dinkelbach's algorithm. The applicability of the models has been demonstrated through two case studies: (i) seawater desalination and (ii) surface water treatment, both for the production of drinking water. The solutions obtained are in a good agreement with existing industrial practices. Comparing the results among the proposed approaches, it can be concluded the proposed MILFP model performs most efficiently in obtaining the best solution with shorter computational times.

Part II

Design and Optimisation of Water Supply Systems

Chapter 4

Design of Water Supply Systems under Hydrological and Allocation Considerations

This chapter zooms out from water treatment to consider the general picture from water withdrawal to supply. It aims at developing a supply system optimisation framework taking into consideration climatic patterns, cost, allocations and trading schemes among market participants.

4.1 Theoretical background

Concurrent population growth, economic development and climate change are the main culprit for the acute and chronic water shortages Morrison et al. [2009], Dizikes [2016], US Environmental Protection Agency [2016]. To mitigate and adapt to the changes, authorities examine strategic options to enhance the supply-demand management for a long term resilience. Planning for 15-35 years ahead by water industries ensures adequate facilities and infrastructure in place to maintain the security of supplies throughout those periods. The gap between supply and demand can be filled by diversifying the portfolio of options for water supply. For instance, alternative sources of water, investing in storage and production capacities, expanding market participants and water quality grade trading options, alongside with interconnectivity and distribution losses minimisation, should be included in the list [Pricewaterhouse Coopers, 2010].

Besides the conventional surface water sources diverted from rivers and lakes, and groundwater extracted from aquifers, non-conventional sources such as seawater, brackish and recycled water have been taking place in the source mix for water provision. Although treated wastewater is not the publicly accepted source for drinking, it is essential for other, non-potable applications in order to meet overall demand. On the other hand, non-conventional sources require more extensive treatment and therefore, more expensive purification techniques hence, they often serve as a back-up during prolonged droughts [Pricewaterhouse Coopers, 2010].

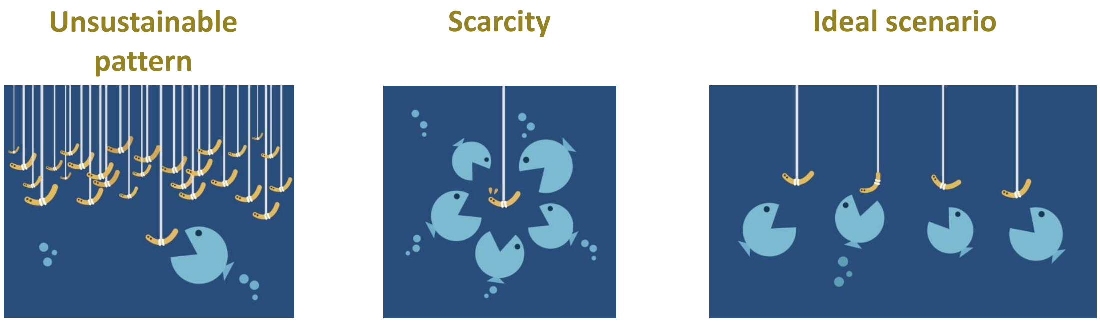


FIGURE 4.1: Resources supply-demand distribution scenarios: unsustainable pattern, when supply exceeds demand (left), scarce pattern, when supply is in deficit (middle) and a sustainable scenario, when supply equals demand (right)

As a limited resource, water usage by an entity can affect its availability to another. Fig. 4.1 demonstrates the three possible patterns, when availability exceeds demand, when demand exceeds availability and when they are equal. The first case results in unsustainable exploitation of resources, the second case demonstrates scarcity, and the third pattern manifests an ideal case scenario when supply is driven by the demand and resources are more evenly distributed among users. Conflict and competition among entities, when it comes to resources, is likely to arise, hence, a coordinated allocation system is sought. Such a system is represented by water markets, operating on the principle of 'cap and trade' system where:

- the cap illustrates the water available for sustainable extraction
- market participants hold water abstraction rights or licences which are a part of the total available pool

- the rights and the allocations in every season can be traded among participants
- the trading price is set by the participants in the water market

Such water trading schemes exist in Spain, Chile, South Africa, Australia, UK and some states in the United States of America. Water market participants may include users such as industry, irrigation operators, urban water utilities, etc. [Australian Government, 2016a]. In a regulated market, the availability of water would govern the extent of trade of an entity with another entity. A thorough way of assessing water availability is by taking into account the environmental flows, such as precipitation, evaporation, run-off, infiltration, etc., shown in Fig. 4.2, which can be expressed by an inflow-outflow water balance for a particular system in a region.

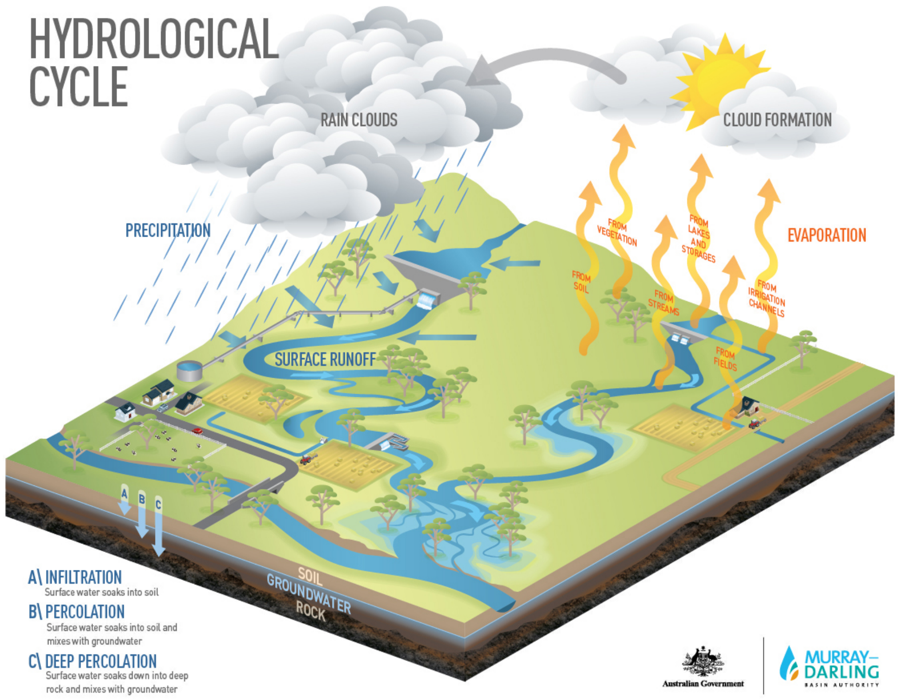


FIGURE 4.2: Hydrological cycle representative scheme showing major inflow and outflow streams accounting towards hydrological balances **Source:** [Australian Government & Murray-Darling Basin Authority, 2016]

Affordable and secure water supply is crucial for the domestic and industrial conduct of daily activities [Zhu et al., 2015]. Water supply reliability can be defined as the probability of meeting demand or the probability of not meeting demand subtracted by one [Hawk, 2003]. Over a time period, reliability becomes the frequency or the quantity of supply shortfalls measured against demand. Governments and water entities, however, are facing numerous challenges providing an adequate supply reliability. Such challenges are climate change, population growth, environmental regulations, decaying infrastructure and calamities. Enhancing trading, and expanding storage and treatment capacities would increase supply reliability [Shamir, 1987, Goulter, 1995, Zhu et al., 2015]. Therefore, satisfactory water management planning and design have to be in place [California Urban Water Agencies, 2012].

Much attention has been paid to optimisation techniques in water supply infrastructure planning as they provide a systematic way of making decisions on future investments. Ray et al. [2010] addressed the issue through a linear programming model for the minimum cost configuration of future water supply, wastewater disposal, and reuse options for the city of Beirut. Koleva et al. [2016b, 2017] proposed linear and non-linear programming models for the optimal design of water and water-related treatment processes. Li et al. [2009] developed a multi-stream, multi-reservoir and multi-period mixed integer linear programming (MILP) model that was integrated into an inexact multistage joint-probabilistic programming to investigate the decision under uncertainty and surplus-flow diversions. Kondili et al. [2010] presented a mathematical framework for the water supply design taking into consideration various sources and users as well as possible conflicting demand over a time period. The model was applied to a case study for the Aegean Islands. Liu et al. [2010, 2011, 2012], Liu [2011], Padula et al. [2013] and Padula [2015] proposed mathematical formulations for the minimisation of proposed installations of plants, storages, pipelines applied on specific case studies. Matrosov et al. [2015] looked at multi-objective optimisation for water supplies focused on London and based on ϵ - dominance non - dominated sorting genetic algorithms and simulation. Saif and Almansoori [2014] suggested a multi-period MILP model for the desalination supply chains with decisions on locations for new and extended plants, storages and pipelines. Al-Nory and Graves [2013] proposed a mathematical programme for the design of desalination supply chain taking into consideration locations of new plants installations. Guerra et al. [2016b] and Saif and Almansoori [2016] integrated water management in different supply chain contexts. Loucks et al. [2005] and Joshi and Joshi [2016] contributed with comprehensive insight into water resources planning, modelling and management and advances in supply systems.

Various works on modelling of water resources allocation and pricing have been published in Brebbia [2015]. Heydari and Qaderi [2015] developed an MILP model for the multi-purpose reservoirs operation. Veintimilla-Reyes et al. [2016] introduced a spatio-temporal mixed integer formulation for water allocation. Yildiran et al. [2015] formulated an MILP model for the short-term scheduling of water reservoirs considering day-ahead market prices. He et al. [2015] proposed an MILP model and applied Benders decomposition method for dynamic resource allocation and traffic assignment in evacuation network. Li et al. [2016] presented a stochastic quadratic model applicable to discrete, fuzzy and random input data for water resources allocation with a case study on Heihe River basin, China. Roozbahani et al. [2015] proposed an approach and a mathematical model for the allocation of water resources among stakeholders. Zeng et al. [2014] constructed a model based on inexact credibility-constrained programming method to investigate the efficiency of water trading under multiple uncertainties. Britz et al. [2013] proposed a Multiple Optimisation Problems with Equilibrium Constraints (MOPEC) for hydro-economic river basin models to account for the decentralised access to water use. Qureshi et al. [2013] introduced a mathematical programming model with an application on agricultural water use in Murray-Darling Basin, Australia. Rinaudo et al. [2016] proposed a price-endogenous model for the trading activity and equilibrium prices in urban water markets. Blanco and Viladrich-Grau [2014] analysed the outcomes of irrigating water trading scheme through a nonlinear mathematical programming model, applied to a case study in Spain. Erfani et al. [2014] presented an optimisation model for short-term pair-wise spot-market trading of surface water rights. It is based on a node-arc multi-commodity approach following a transaction tracking method [Erfani et al., 2013]. Peng et al. [2015] proposed an optimisation model for water transfer decision making process considering shortages in reservoirs of both, recipients and donors.

In the light of the increasing stress on water resources, their planning should no longer be based on a single-dimensional analysis. Instead, decision making needs to entail the economically viable infrastructure design in climatic, regulatory and reliability contexts. To the best of the author's knowledge, no work addresses this necessity. The chapter addresses this gap by not only combining all the aforementioned separate concepts but also considering the entire water cycle with legislative regulations altogether in a mixed integer linear programming (MILP) formulation. The chapter, thus, aims at investigating how to consolidate those multiple-aspects into a single optimisation framework. A multiple number of sources, users, trading and time periods are geographically considered. The locations and capacities for surface, groundwater, seawater plants and the trading volumes of each source among regions are to be optimised.

The rest of this chapter is structured as follows: Section 4.2 sets out the problem statement whose mathematical formulation is presented in Section 4.3. The applicability of the model is investigated in a case study, described in Section 4.4, followed by results and discussion in Section 4.5. Finally, concluding remarks are made in Section 4.6.

4.2 Problem statement

The supply system problem at hand entails strategic decisions for the allocation of water resources, procurement and treatment of sources types, locations and capacities augmentations for dams and treatment plants, trading directions and volumes.

A geographical area is considered where water demands can be met by surface water, groundwater and seawater. Options such as reclaimed water and individually collected storm water are disregarded in this work. The area is divided into sub-regions, or states, based on their federal governance and autonomy. The water demand for each territory is estimated according to the population predictions and consumption patterns per capita. Additionally, the water demand varies seasonally, peaking in summer and plummeting in winter. Spring and autumn seasons are characterised with moderate consumption volumes. Regulated water services of every region are provided by water suppliers to meet the urban water demand, which occurs from residential, commercial, municipal and industrial usage. A state might not be able to meet its regional demand consequently, it should identify a strategy for dealing with water deficit. In case source water is in deficit, trading among regions is considered. On the other hand, if storage or production capacities are not sufficient, optimal decisions for the capacity and location for the expansion of existing plants, and installation of new dams and plants are made.

Water is diverted from lakes and reservoirs, and abstracted from aquifers taking into account the seasonal hydrological cycles and sustainable yields (withdrawals) within the territories. Water balances, or budgets, are performed over the total regional available water storages. Reservoirs, dams, ponds, lakes and groundwater aquifers are referred to as storages. The inflows into the storages are the seasonal precipitations, run-off, streamflows and recharge while the outflows consist of evaporation, discharge and diverted/abstracted volumes. Precipitation refers to the rainfall that falls directly onto the storage area. Run-off represents excess of moisture turning into the streamflow from the catchments or drainage basins to the storage. Streamflows refer to the river flowing into the storage. Evaporation is the direct evaporation from the storage surface, while discharge refers to the river stream leaving the system. Diversions are the water flows withdrawn for human usage. Groundwater discharge or seepage is ignored due to the scarce historical data available. As a matter of convenience, the streamflows for different river systems in a region have been summed up. It is assumed that dead storage comprises 10% of the water storage capacity. Further, by a rule of thumb, 10% of the rainfall in drainage basins infiltrates to become groundwater inflow. Climatic data is extracted for the entire planning horizon reflecting fluctuations in the weather conditions and mimicking el Niño and la Niña events, which occur every 5-7 years. Oceans and seas are not taken into account in water budgets due to their abundance.

In every region there are rights for maximum water sources diversions/extractions. They are called target allocations, or entitlements, and apply for surface water and groundwater. In a season when availability in storage is sufficient, the allocations in a region can reach target allocations. The amount of water that has been allocated for withdrawal and has not been used in a given year can be rolled to the next year unless regulations oblige a return to the abstraction basin. After the resources are withdrawn, they are processed in surface water treatment plants (SWTP), groundwater treatment plants (GWTP) and seawater desalination plants (SDP) which operate with different efficiencies. Then, the product water is distributed for urban usage, after which it is assumed 60% of that water is collected as sewerage. The wastewater is then treated in wastewater treatment plants (WWTP) and returned as recharge. It must be noted that no decisions are made with respect to WWTPs and the concept is introduced merely to close the water cycle. A scheme, representing the problem, is illustrated in Fig. 4.3.

Assumptions

- Dead storage accounts for 10% of total storage
- Percolation accounts for 10% of the land rainfalls
- Outflow and moving of groundwater is disregarded
- Self-supplied water and recycled water to meet urban demand are disregarded
- Purification plants operate 300 days a year
- Efficiencies of plants are adopted based on their treatment technologies
- 60% of the water supplied is collected in sewage
- Historic traded volumes and prices apply for state water providers
- Trading occurs for regions sharing a basin or being connected through a pipeline
- No carry-over clearance, i.e. in every year it is allowed to carry allocations over

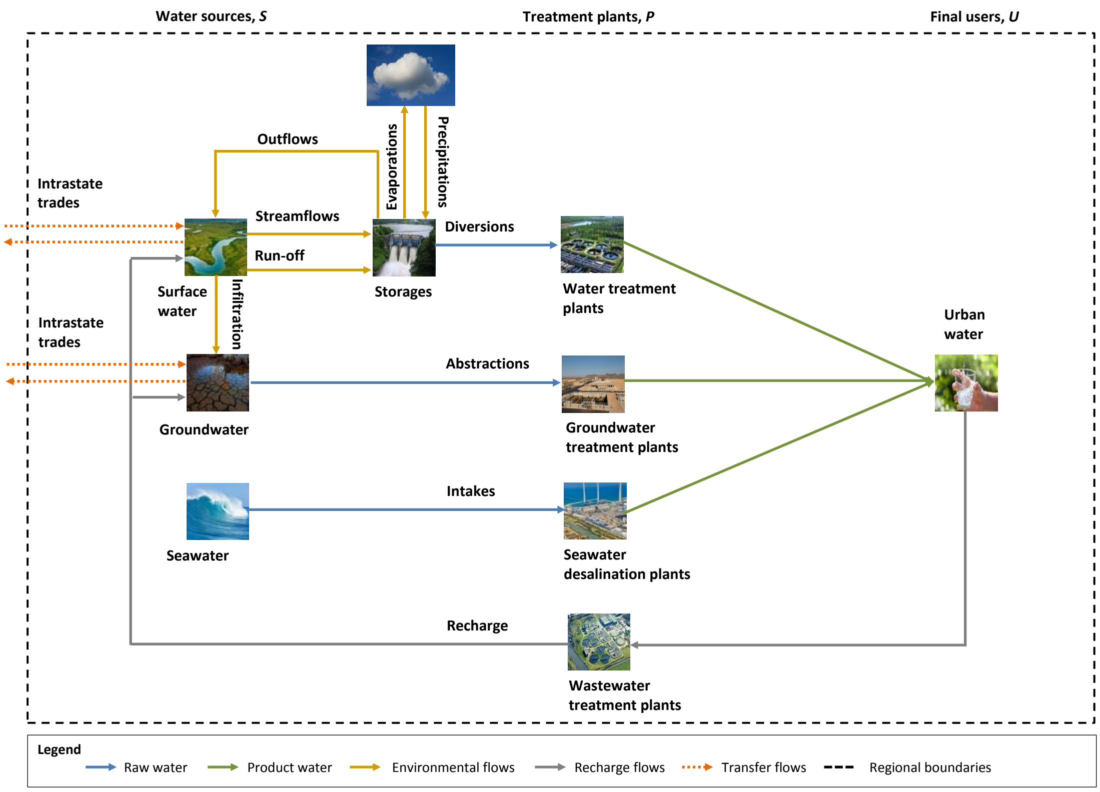


FIGURE 4.3: Schematic representation of the water network system

Thus, the problem description with key parameters can be stated below.

Given:

- geographical divisions into regions/states/territories
- planning time horizon, e.g. a 25 - year horizon
- water sources, i.e. surface water, groundwater, seawater, etc.
- final water uses, i.e. urban, rural, etc., and seasonal demand over planning horizon
- regional and seasonal climatic data, i.e. precipitation, evaporation, run-off, streamflows
- initial water storages in drainage basins and reservoirs
- geographical distribution, capacities, operating efficiencies, and operating and capital cost parameters of existing and potential dams and plants
- maximum allocated water sources per end-use, i.e. entitlements
- trading topology and prices options
- inflation and discount factors
- regional sustainable diversions/abstractions
- penalty costs for not meeting demand

Determine:

- available water sources for diversion/abstraction
- procurement rate for each water source and end-use water production rate
- trading and carry-over flowrates
- water supply reliability
- location and capacities of new dams and plants installations, and existing plants expansions

So as to: to minimise the annualised total cost for operating and building the network proposed subject to environmental, operational, logical and economic constraints. The supply system problem is formulated as a spatially-explicit multi-period Mixed Integer Linear Programming (MILP) model.

4.3 Mathematical formulation

In this section the mathematical formulation is presented as a single objective problem, where key constraints are the water cycle balances, procurement and production constraints, logical constraints, supply reliability, and operating and capital expenditures. The objective is to minimise the total cost for the entire region within the planning horizon.

4.3.1 Hydrological balances

The estimation of water availability in storage rests on the inflows into the system, R_{igtq}, recharges, RC_{igtq} and the total storage from the previous season, $S_{igt,q-1}$. RC_{igtq} are the flows returned to nature after having been collected from users and treated. R_{igtq} represents a summation of rainfall, run-off and streamflows for surface water, and infiltrated rainfall for groundwater, shown in Eq.(4.1) and Eq.(4.2).

$$R_{igtq} = R^{ain}_{igtq} + R^{unoff}_{igtq} + R^{iver}_{igtq}, \forall i = "sw", g, t, q \tag{4.1}$$

where R^{ain}_{igtq} is the direct rainfall to the reservoir, R^{unoff}_{igtq} is the run-off seeping into the reservoirs and R^{iver}_{igtq} represents the stream inflows to the storage. It is assumed that run-off occurring in one region fills the reservoirs in the same region and no other neighbouring regions. It must be noted that run-off data have been collected through personal communication with the Australian Water Assessment Modelling Section of the Bureau of Meteorology. A proportion of the rainfall which falls onto the mainland, LR^{ain}_{igtq}, infiltrates into the ground and becomes an inflow for aquifers.

$$R_{igtq} = r^{infl} \cdot LR^{ain}_{igtq}, \forall i = "gw", g, t, q \tag{4.2}$$

where r^{infl} is the fraction of the rainfall that infiltrates. Simultaneously, the total outflows from the system are the evaporation losses, L_{igtq}, outflows, O_{igtq} and allocated water, A_{igtq}. It is assumed no additional losses occur for both, surface water and groundwater systems. The inflows and outflows are illustrated in Fig. 4.4. The seasonal and yearly formulations are shown in Eq. (4.3) and Eq. (4.4), respectively.

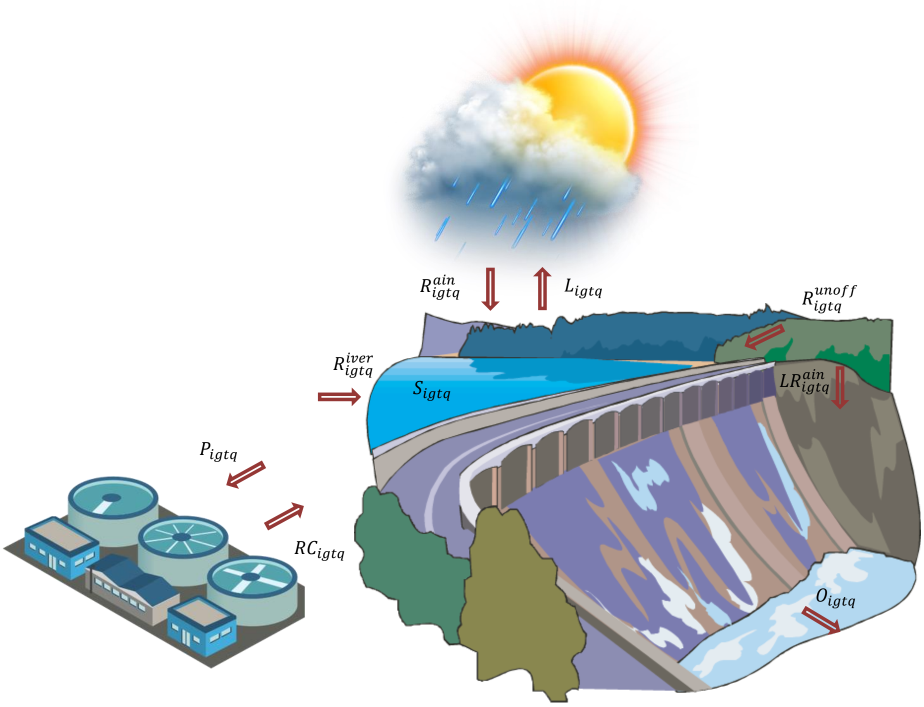


FIGURE 4.4: Inflows (rainfall, run-off, river streamflows, recharges) and outflows (evaporation, withdrawals, outflows) from a reservoir system

$$\begin{aligned} DS_{igtq}|_{i=\text{"}sw\text{"}} + WS_{igtq} = DS_{igt,q-1}|_{i=\text{"}sw\text{"}} + WS_{igt,q-1} + R_{igtq} + RC_{igtq} + \\ AC_{igtq} - L_{igtq}|_{i=\text{"}sw\text{"}} - A_{igtq} - O_{igtq}|_{i=\text{"}sw\text{"}}, \\ \forall i \in LW, g, t, q > 1 \end{aligned} \tag{4.3}$$

$$\begin{aligned} DS_{igtq}|_{i=\text{"}sw\text{"}} + WS_{igtq} = DS_{ig,t-1,q}|_{i=\text{"}sw\text{"},q=4} + WS_{ig,t-1,q}|_{q=4} + R_{igtq} + RC_{igtq} + \\ AC_{igtq} - L_{igtq}|_{i=\text{"}sw\text{"}} - A_{igtq} - O_{igtq}|_{i=\text{"}sw\text{"}}, \\ \forall i \in LW, g, t, q = 1 \end{aligned} \tag{4.4}$$

where LW is a set containing the inland water sources, i.e. surface water and groundwater. Surface water storages include dams, and natural storages, i.e. lakes and wetlands. In this work, a cumulative term to refer to both, human-made and natural storages, is storage or reservoir. Aquifers are the only storage for groundwater which occurs in its natural form. The sum of dams' storage, DS_{igtq}, and natural storage, WS_{igtq} add up to the total storage, S_{igtq}, shown in Eq. (4.5).

$$S_{igtq} = DS_{igtq}|_{i=\text{"}sw\text{"}} + WS_{igtq}, \forall i \in LW, g, t, q \tag{4.5}$$

where at $t = 0$ and $q = 0$ the storage is the summation of the initial reservoirs' and lakes' storages. A representation of the time disretisation in years, seasons and their sequence is demonstrated in Fig. 4.5.

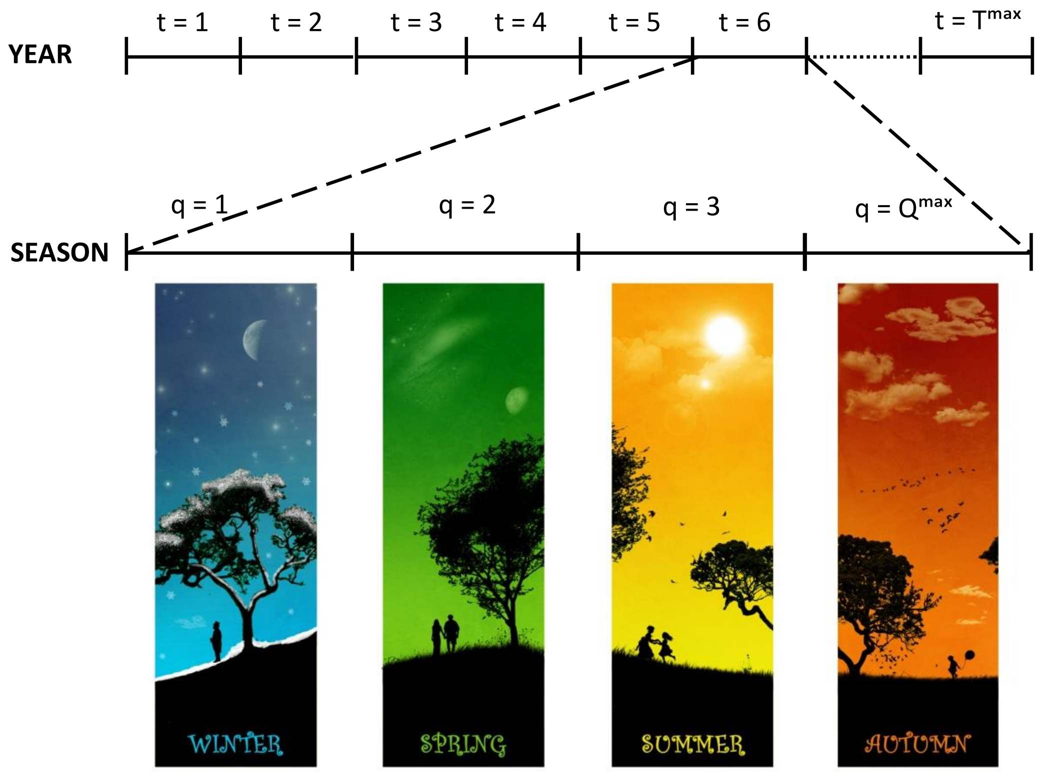


FIGURE 4.5: Visualisation of year and seasonal time discretisation. The sequence of seasons q depends on the start and end of the fiscal year t a government uses

The maximum natural storage capacity per region, WS_{ig}^{max}, should not be exceeded in any year t and season q in order to prevent overflows (Eq. (4.6)).

$$WS_{igtq} \leq WS_{ig}^{max}, \forall i = \text{"}sw\text{"}, g, t, q \tag{4.6}$$

4.3.2 Supply - demand balances

Fig. 4.6 delineates the water supply system flows for given regions g and g'.

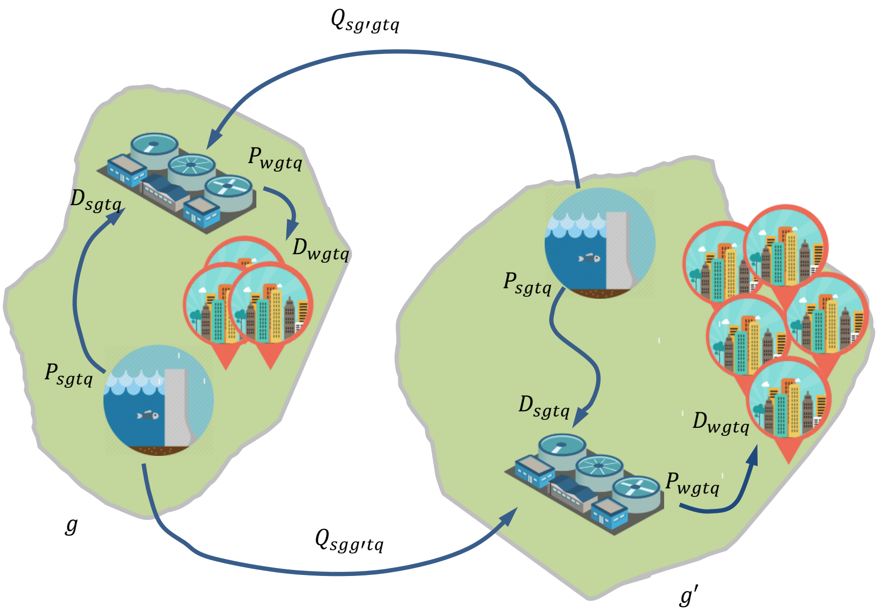


FIGURE 4.6: A supply-demand flow diagram, including withdrawals, production, distribution and trading between region g and region g'

Eq.(4.7) represents those interactions through a global mass balance equation which entails the water type flows i ($I = S \cup W$) at every node of the WSC: withdrawals of raw water s, P_{sgtq}, according to purification plant intake demand, D_{sgtq}, and production of final grade water w, P_{wgtq}, to meet populated centres demand, D_{wgtq}. It also takes into account $Q_{igg'tq}$ and $Q_{ig'gtq}$, which are the traded flows sent to and received from other regions, respectively.

$$D_{igtq} + \sum_{g' \in \eta_{igg'}} Q_{igg'tq} - PD_{igtq} = P_{igtq} + \sum_{g' \in \eta_{ig'g}} Q_{ig'gtq}, \ \forall i, g, t, q \tag{4.7}$$

where $\eta_{igg'}$ and $\eta_{ig'g}$ define the allowed directions of flow from region to region. Regions with hydrological or physical connectivity are selected for trading. When a demand cannot be met by the treatment plants, water flows, PD_{igtq}, are allowed to compensate for the shortage. These flows are penalised in the objective function.

4.3.3 Procurement constraints

The amounts of diverted surface water and extracted groundwater are determined by the allocated water rights, or allocations A_{igtq}, a region g is allowed to withdraw in year t and season q. The carry-over volumes, AC_{igtq}, are the amounts rolled over from one season to the next after ensuring enough water is set aside for meeting the regional demand. The seasonal and annual expressions are shown in Eq.(4.8) and Eq.(4.9), respectively.

$$AC_{igtq} = AC_{igt,q-1} + A_{igtq} - P_{igtq}, \forall i \in LW, g, t, q > 1 \tag{4.8}$$

$$AC_{igtq} = AC_{ig,t-1,q}|_{q=4} + A_{igtq} - P_{igtq}, \forall i \in LW, g, t, q = 1 \tag{4.9}$$

The central principle behind carry-over is that unused water can be carried over, but it must not displace inflows that support new allocations. Only inland water LW is affected by allocation rules due to the associated finiteness with those resources. The allocations are calculated on the basis of the water rights, or the entitlements ent_{igt}, which are the maximum water volumes that can be withdrawn in year t.

$$\sum_{q} A_{igtq} \leq ent_{igt}, \forall i \in LW, g, t \tag{4.10}$$

The entitlements are treated as parameters based on the assumption that they are automatically renewed from year to year. In this work, it is assumed that maximum 100% of the entitlements can be received in a year t.

Additionally, a limitation is considered that a region g can trade water with other regions g' only when g satisfies its regional demand from the seasonal allocations available (Eqs. (4.11)-(4.13)).

$$\sum_{g' \in \eta_{igg'}} Q_{igg'tq} \leq ent_{igt} \cdot B_{igtq}, \forall i \in LW, g, t, q \tag{4.11}$$

$$P_{igtq} \leq D_{igtq} + ent_{igt} \cdot B_{igtq}, \forall i \in LW, g, t, q \tag{4.12}$$

$$P_{igtq} \geq D_{igtq} - ent_{igt} \cdot (1 - B_{igtq}), \forall i \in LW, g, t, q \tag{4.13}$$

where B_{igtq} is a binary variable, equal to 1 when demand for a source i in a region g is lower than the supply. Further, the diverted or abstracted volumes should be within the limit of sustainable withdrawals, recommended by local governments (Eq.(4.14)).

$$\sum_{q} P_{igtq} \leq SP_{igt}^{max}, \forall i = LW, g, t \tag{4.14}$$

where SP^{max}_{igt} is the maximum sustainable water diversion or abstraction in a year t. These limits are in place to ensure the withdrawn volumes would not exhibit a detrimental impact on the environment.

4.3.4 Reliability of water supply

It is a common practice in many cities to be under agreed volumetric or temporal water restrictions, or an agreed reliability of supply. The reliability of water supply is calculated based on the volumetric shortage, when the demand exceeds supply. The water supply reliability, WSR_{igtq}, is shown in Eq.(4.15).

$$WSR_{igtq} = 1 - PD_{igtq}/dem_{igtq}, \forall i \in W, g, t, q \tag{4.15}$$

where PD_{igtq} is the import in a period of water shortage and dem_{igtq} is the urban water demand. The normalised reliability for the entire country is an average of the regional reliabilities (Eq. (4.16)).

$$WR = \sum_{i \in W} \sum_{g} \sum_{t} \sum_{q} WSR_{igtq}/(G^{max} \cdot T^{max} \cdot Q^{max}) \tag{4.16}$$

where WR is the normalised reliability, T^{max} is the planning horizon period, Q^{max} - the number of seasons and G^{max} is the total number of regions.

4.3.5 Capacity constraints

At a given time t, every region g and plant p have production capacity, $TCAP_{gpt}$, which is a limiting factor for the plant feed flow, V_{igptq}. Therefore, the effluent should not exceed the total plant capacity, demonstrated in Eq.(4.17).

$$\sum_{i \in S \cap SP_p} \sum_{i' \in W} \epsilon_{ii'} \cdot V_{igptq} \leq TCAP_{gpt}/Q^{max}, \forall g, p \in PG_g, t, q \tag{4.17}$$

where $\epsilon_{ii'}$ is the production yield, depending on water source i. PG_g is a subset of g which contains the operating plant p in region g, and Q^{max} is the number of seasons used to obtain seasonal capacity. Provided more water has to be processed to meet demand, the total capacity will increase by installing new plants or expanding old ones. A binary variable I_{gplt} is assigned for the installation of new plant p with capacity l in region g at time t. When an increase in capacity is necessary, I_{gplt} is activated and equals 1, otherwise it equals 0. Another binary variable, E_{gplt}, is assigned for the expansion of existing plants, which operates on the same principle.

$$TCAP_{gpt} = TCAP_{gp,t-1} + \sum_{l} icap_{pl} \cdot I_{gpl,t-ict_p}|_{p \in NP} + \sum_{l} ecap_{pl} \cdot E_{gpl,t-ect_p}, \quad \forall g, p \in PG_g, t \tag{4.18}$$

where ict_p and ect_p are the respective construction and expansion times for plant p, $ecap_{pl}$ represents the available options of capacity expansion l and $icap_{pl}$ - the capacity installation options of new plants (NP) throughout the planning horizon. At most one capacity level l from a given number of options can be chosen (Eq.(4.19)).

$$\sum_{l} \sum_{t} I_{gplt} \leq 1, \forall g, p \in PG_g \cap NP \tag{4.19}$$

E_{gplt} is a binary variable that is active when a plant is expanded which can happen up to E^{max} number of times (Eq. (4.20)).

$$\sum_{l} \sum_{t} E_{gplt} \leq E^{max}, \forall g, p \in PG_g \tag{4.20}$$

Only one capacity level l from a given number of options can be chosen to be expanded at a time (Eq.(4.21)).

$$\sum_{l} E_{gplt} \leq 1, \forall g, p \in PG_g, t \tag{4.21}$$

Expansions can occur only after a plant has been installed, imposed by Eq.(4.22).

$$\sum_{l} E_{gplt} \leq \sum_{l} \sum_{t' \leq t - ict_p} I_{gplt'}, \forall g, p \in PG_g \cap NP, t \tag{4.22}$$

The surface water that is kept in dams' storage should be less or equal than the current existing dams' capacity.

$$DS_{igtq} \leq DAM_{gt}, \forall i = "sw", g, t, q \tag{4.23}$$

In Eq.(4.23), DAM_{gt} is the total capacity of dams in every region g at time t. As DS_{igtq} is the water volume related to the ability to withdraw water from it, the volume of water which stagnates should be considered. Hence, simultaneously, the storage should not fall below the dead storage of the reservoir, expressed in Eq.(4.24).

$$DS_{igtq} \geq dsf \cdot DAM_{gt}, \forall i = "sw", g, t, q \tag{4.24}$$

where dsf is a factor for the typical dead storage which remains in dams. The total dams capacity in a region equals the capacity of the existing dams and the newly built dams. The decision of building a new dam is executed through a binary variable ID_{glt}.

$$DAM_{gt} = DAM_{g,t-1} + \sum_{l} idam_{gl} \cdot ID_{gl,t-dct}, \forall g, t \tag{4.25}$$

where dct is the time for dam construction and $idam_{gl}$ represents the option l for capacity installation of dams in region g. Only one capacity option l can be selected in a region g, given in Eq.(4.26).

$$\sum_{l} \sum_{t} ID_{glt} \leq 1, \forall g \tag{4.26}$$

4.3.6 Production constraints

The water flows that are withdrawn to be processed in plants must equal the demand for raw sources, D_{igtq}, calculated from Eq.(4.27).

$$D_{igtq} = \sum_{p \in SP_i \cap PG_g} V_{igptq}, \forall i \in S, g, t, q \tag{4.27}$$

The above equation applies only to raw sources, S, i.e. surface water, groundwater and seawater. The production of water for usage, P_{igtq}, equals the summation of the effluents from plants treating different raw waters (Eq.(4.28)).

$$P_{igtq} = \sum_{i' \in S} \sum_{p \in SP_{i'} \cap PG_g} \epsilon_{i'i} \cdot V_{i'gptq}, \forall i \in W, g, t, q \tag{4.28}$$

The regional user demand, dem_{igtq}, must be met and this condition is enforced from the equation below.

$$(1 - dff_g) \cdot D_{igtq} = dem_{igtq}, \forall i \in W, g, t, q \tag{4.29}$$

where the equation applies only for final product water purpose W. The parameter dff_g accounts for the distribution losses due to broken pipes and leakages varying regionally.

The recharge volumes, RC_{igtq}, are estimated by the amount of water that has been collected in sewerage, treated by wastewater treatment plants and returned to surface and groundwater storages (Eq.(4.30)).

$$RC_{igtq} = \sum_{i' \in W} up \cdot \epsilon_{i'i} \cdot D_{i'gtq}, \forall i \in LW, g, t, q \tag{4.30}$$

where up is the water utilisation percentage, i.e. the fraction of distributed water which is collected as sewage, and $\epsilon_{i'i}$ is the operating efficiency of the wasterwater treatment plant.

4.3.7 Operating expenditure constraints

The operating expenditures are calculated in a similar manner. The operating costs for maintaining the dams, $ODAM_t$, are calculated by Eq.(4.31).

$$ODAM_t = \sum_{g} vod_t \cdot DAM_{gt}, \forall t \tag{4.31}$$

where vod_t are the variable operating costs of dams at time t. The operating costs of plants consist of fixed, fop_{plt} and variable, vop_{plt} costs (Eq.(4.32)).

$$\begin{aligned} OPL_t = & \sum_{p \in OP} \sum_{l} fop_{plt} + \sum_{g} \sum_{p \in PG_g \cap NP} \sum_{l} fop_{plt} \cdot IP_{gplt} + \\ & \sum_{g} \sum_{p \in PG_g} \sum_{l} \sum_{i : p \in SP_i} \sum_{i' \in W} \sum_{q} vop_{plt} \cdot \epsilon_{ii'} \cdot V_{igptq}, \ \forall t \end{aligned} \tag{4.32}$$

The penalised cost for not meeting the product water demands is calculated by Eq.(4.33).

$$OPen_t = \sum_{i \in W} \sum_{g} \sum_{q} pc \cdot PD_{igtq}, \forall t \tag{4.33}$$

where pc is a penalty cost rate, chosen as a number, significantly higher than trading costs. The total OPEX is a summation of the operating dams' and plants' costs and trading costs, expressed from Eq.(4.34).

$$OPEX_t = ODAM_t + OPL_t + OTR_t, \forall t \tag{4.34}$$

4.3.8 Capital expenditure constraints

Next, the capital expenditure for dams, plants installation and expansion is discussed. The CAPEX of dams, $CDAM_t$, depends on the capacity option l for installation selected and the corresponding cost for construction, $capdam_l$ (Eq.(4.35)).

$$CDAM_t = \sum_{g \in ND} \sum_{l} capdam_l \cdot ID_{glt}, \ \forall t \tag{4.35}$$

The capital cost of plants, CPL_t, is a summation of the costs for installations and expansions, and is calculated from Eq.(4.36).

$$CPL_t = \sum_{g} \sum_{p \in PG_g \cap NP} \sum_{l} caplant_{pl} \cdot I_{gplt} + \sum_{g} \sum_{p \in PG_g} \sum_{l} capexp_{pl} \cdot E_{gplt}, \ \forall t \tag{4.36}$$

where $caplant_{pl}$ and $capexp_{pl}$ are the capital costs associated with a plant p and its respective installed or expanded capacity l. The total capital cost is the sum of all the capital cost components and is shown in Eq.(4.37).

$$CAPEX_t = CDAM_t + CPL_t, \ \forall t \tag{4.37}$$

where $CAPEX_t$ is the capital expenditure at time t.

4.3.9 Objective function

The total cost, TC, represents the addition of the capital, operating costs and penalty over the planning time horizon (Eq.(4.38)).

$$minimise \ \ TC = \sum_{t} (cdf_t \cdot CAPEX_t + odf_t \cdot OPEX_t + odf_t \cdot OPen_t) \tag{4.38}$$

where cdf_t and odf_t are discount factors of the capital and operating costs, respectively. The objective function is subject to:

- hydrological and supply-demand balances Eq.(4.3) - Eq.(4.7)
- procurement constraints Eq.(4.8) - Eq.(4.14)
- reliability constraints Eq.(4.15) - Eq.(4.16)
- capacity constraints Eq.(4.17) - Eq.(4.26)

- production constraints Eq.(4.27) - Eq.(4.30)
- operating expenditure constraints Eqs.(4.31),(4.32), Eq.(4.33) - Eq.(4.34)
- capital expenditure constraints Eq.(4.35) - Eq.(4.37)

Next, the mathematical formulation is tested on a specific problem, explained in Section 4.4.

4.4 Illustrative example

The applicability of the proposed framework is investigated on a case study about Australia. The objective is to minimise the total country's cost for obtaining an optimal water network by meeting the regional urban water demands. In this section, the major data on regional divisions, water demands, efficiency factors, hydrological data, installation and expansion capacities, and cost factors are presented.

4.4.1 Geographical representation of Australian regions

Australia is divided into 8 internal state and territory governments, namely: Queensland (QLD), New South Wales (NSW), Victoria (VIC), South Australia (SA), Western Australia (WA), Northern Territory (NT), Australian Capital Territory (ACT) and Tasmania (TAS). Each state has its local state government which owns all or most of the water providers operating within the state [Australian Government, 2017]. Australian water providers can supply urban and rural areas with drinking as well as different quality grades water. Due to the large number of providers and the available data on regional water demand and hydrological balances, the spatial discretisation is performed on a state basis. Besides water supply, the majority of the suppliers offer sewerage management, too. A map showing the considered regions is shown in Fig. 4.7.

4.4.2 Existing plants and dams for providing urban water supply

Each state possesses assets for the treatment of any of the three sources considered: seawater, surface water and groundwater.

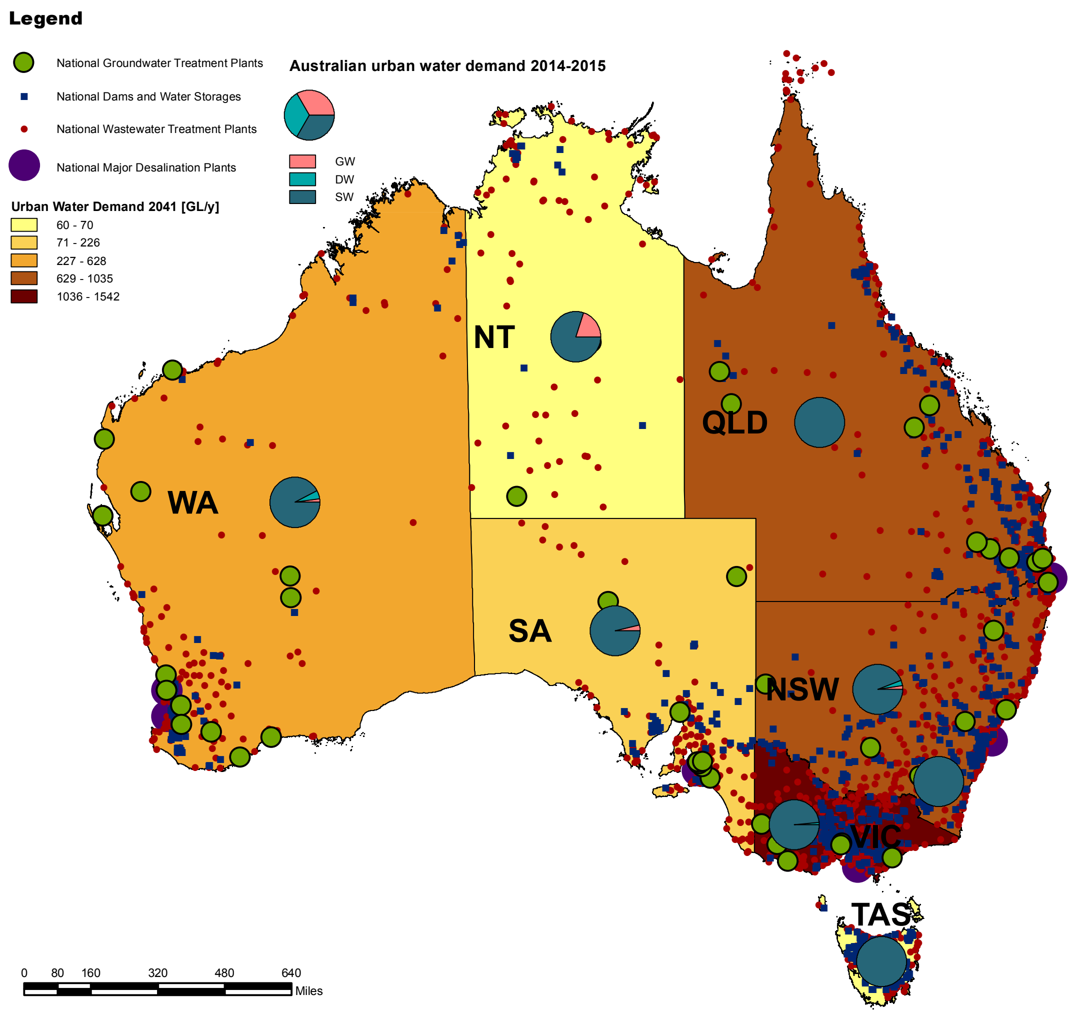


FIGURE 4.7: Dams, major plants and urban water demand and source mix in Australia

The prolonged lack of rainfall from 2000 - 2010 in Australia necessitated finding alternative sources of water supply. Seawater desalination, although an expensive option, has been considered as the leading solution to water shortages. Currently, in every state but TAS, NT and ACT exists at least one large capacity seawater desalination plant (Fig. 4.7). Their locations, capacities and construction costs are summarised in Table 4.1. The plants are in operation as a non-conventional measure in drought periods, when there is insufficient freshwater in the states' storages. In 2016 all desalination sites were producing drinking water.

Groundwater in Australia is extracted from underground aquifers and after the appropriate treatment it can be used for water supply, agriculture and industry. Its salinity

TABLE 4.1: Seawater desalination plants, locations, capacities and cost

Name	State	Max capacity [ML/d]	Construction cost [M USD]
Gold Coast Desalination Plant	Queensland	167	912
Perth Desalination Plant	Western Australia	130	294
Kurnell Desalination Plant	New South Wales	500	1,444
Southern Seawater Desalination Plant	Western Australia	290	726
Victorian Desalination Plant	Victoria	550	2,660
Port Stanvac Desalination Plant	South Australia	270	1,391

source: Australian Government [2016b]

can be high enough to be considered for brackish water and hence, its purification can sometimes be referred to as brackish water desalination. States that count on groundwater availability are Western Australia and the Northern Territory due to their remoteness from the main river basin - Murry - Darling. Fig. 4.7 depicts the locations of the larger groundwater treatment plants in Australia.

Dams can be defined as "an artificial barrier that has the ability to impound water, wastewater, or any liquid-borne material, for the purpose of storage or control of water" [International Commission on Large Dams, 2016]. They can vary immensely in size and shape, from small dams that serve for watering farms to large dams that can provide the storage for urban centres. In Australia there are altogether more than 600 dams numbering a total capacity of approximately 80,000 GL. A spatial representation of all Australian dams' locations is shown in Fig. 4.7. The cumulative capacity of all dams in a state is reported in Table 4.2.

TABLE 4.2: Demand - supply regional data

	Accumulative dams' capacity [GL]	Urban water consumption per capita [kl/year]	Distribution losses [%]
SA	2,257	125	11.9
VIC	12,864	188	7.9
NSW	21,352	104	11.1
QLD	10,429	123	12.0
ACT	158	102	7.2
NT	285	211	19.5
WA	11,474	136	22.0
TAS	22,141	112	36.4

source: Australian Bureau of Statistics [2015a,b]

Surface water in Australia is diverted from lakes, rivers and streams and dams, and its abstraction volumes depend on the precipitation in the territories. Tasmania possesses sufficient amounts of freshwater whereas SA, VIC, QLD and NSW rely predominantly on the availability in Murry - Darling Basin (MDB). The availability of freshwater in

WA and NT is limited. Surface water treatment plants may involve full treatment with coagulation and filtration or membrane purification, or only chlorination or UV disinfection. In the former case, the facilities have maximum capacity while in the latter one, the reservoirs capability to supply water is considered. A full list of entities is provided in the supplementary material of this manuscript.

4.4.3 Urban water sources and demands

In Fig. 4.7 the percentage of the different water source origins per state used for urban water supply in 2014-2015 are shown. It can be deduced from the figure that the eastern territories rely mostly on surface water due to the presence of Murray Darling Basin (MDB) while the territories to the west and north provide their urban water by treating groundwater from aquifers and desalinating seawater [Australian Bureau of Statistics, 2015b]. The desalination plants in QLD, VIC and NSW were on a stand-by mode for the period. Additional source origin-related assumptions in this work include: (i) self-supplied and reuse water are not accounted for, and (ii) surface water treatment, and groundwater and seawater desalination provide the majority of the urban water supply.

The consumption of urban water comes from residential, commercial, municipal and industrial water usage [Planning Institute Australia, 2016]. Its projections heavily depend on population growth, climate change, type of houses, economic growth, water efficient appliances, demographics, etc. The total urban water resources predictions are calculated by multiplying the projected population by the consumption per capita, which, on the other hand, is a quotient of the urban water demand and population in the base year of calculation (2014). The regional consumption per capita is given in Table 4.2. It is assumed the consumption rate does not alter from the patterns observed in 2014 [Australian Bureau of Statistics, 2015a]. Population projections follow three scenarios: a high, medium and low one. The medium scenario is seen as the most probable course and therefore, the scenario used as a prediction in the case study. Interpolation was used to determine the population between 2026 and 2030 for Western Australia. The derived urban water demand predictions are illustrated in Fig. 4.8.

The population projections for Victoria and Queensland indicate approximately a 47% and 56% respective increase and consequently, affecting the predicted water consumptions in those states with the same estimated percentage. Almost insignificant change

FIGURE 4.8: Predicted urban water demand from 2016 to 2041

in the predicted consumption in ACT, SA, TAS and NT is seen as a relatively steady population expected for that period. The highest consumption at the end of the planning horizon would be in VIC, where the demand will reach approximately 1,550 GL in year 2041.

The seasonal variation in demand is also considered where water consumption in summer is approximately twice as much as consumption in winter, whereas spring and autumn are characterised with moderate demands. The assumption follows the outcome of studies for urban water use varying with seasonal rainfall and temperatures [Maidment et al., 1985].

A high percentage from the urban water, which has been distributed, is lost due to leakages, broken pipes, etc. The percentage varies for different states as shown in Table 4.2 [Australian Bureau of Statistics, 2015b].

4.4.4 Hydrological data

Climate in Australia varies from year-to-year due to the shifting and alternating extensive dry and wet patterns in the Pacific Ocean. The phenomena refer to El Niño and La Niña and cause prolonged droughts occurring every three to eight years followed by prolonged rainfalls occurring with the same frequency [Australian Bureau of Meteorology, 2008]. Consequently, hydrological components, which determine the availability of water, are affected. The water cycle, or budget, is a balance of the inflows, outflows and changes in storage within a geographic area, or catchment. In this case study, the inflows, which are given as data, are rainfalls, run-off and streamflows, and the outflow, given as data, is evaporation.

Regional seasonal changes in the rainfall and pan evaporation are considered, where depicted in Fig. 4.9 and Fig. 4.10 are the total values for Australia for the period 2016-2041. The data are the recorded historical data per state which is available from the Australian Bureau of Meteorology [Australian Bureau of Meteorology, 2016a,b]. Pan evaporation is the evaporation that occurs in a pan and therefore, has to be corrected with a correction factor which can range between 0.47 and 1.18 [Finch and Calver, 2008]. A value of 0.75 is adopted in this case study. Australian summer takes place in months January - March, autumn in April - June, winter in July - September and spring in October - December. The largest numbers for precipitation and evaporation are recorded in autumn and winter while both decrease in the spring and summer seasons.

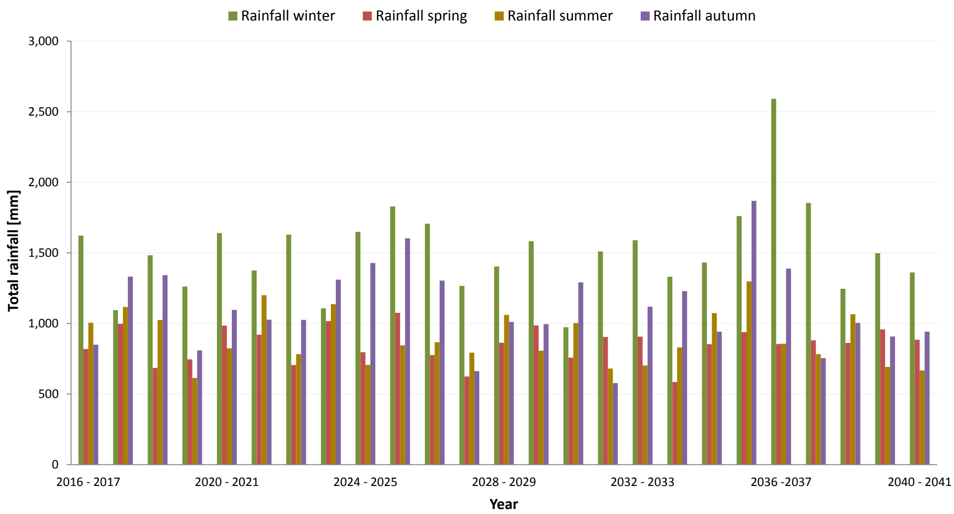


FIGURE 4.9: Total seasonal rainfall in the period 2016 - 2041

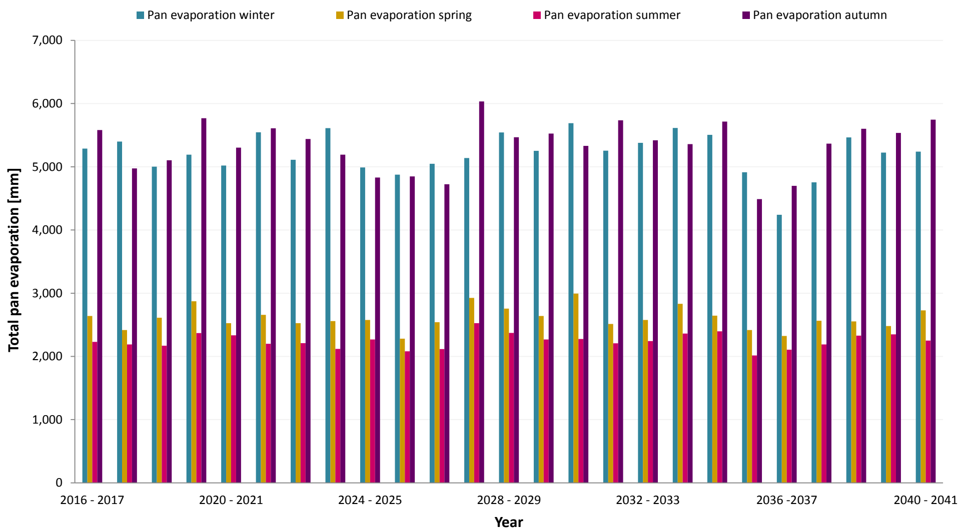


Figure 4.10: Total seasonal pan evaporations in the period 2016 - 2041

Run-off is taken from personal correspondence with the Bureau of Meteorology. Infiltration is the recharge inflow to groundwater and is a fraction of the rainfall. A worst-case scenario of 10% recharging aquifers is assumed [American Planning Association, 2006].

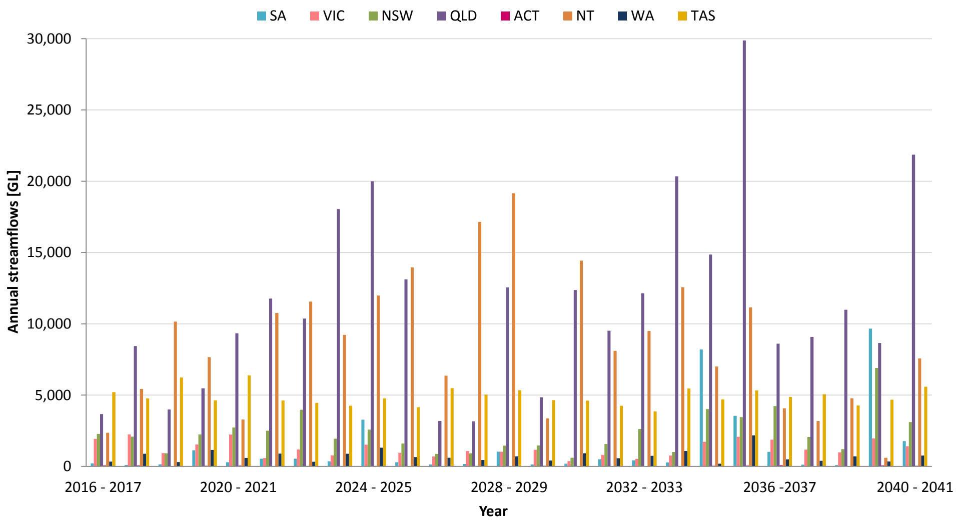


Figure 4.11: Total seasonal streamflows in the period 2016 - 2041

The streamflows data have been collected from the official site of the Australian Bureau of Meteorology Australian Bureau of Meteorology [2016c] where all the major rivers gauged historical flowrates were recorded. The flows from different river systems were added up. It can be observed from Fig. 4.11 that the volumes of the streams follow rainfall trends. The data is processed per region but the total streamflows in a given period are depicted in the figure.

TABLE 4.3: Initial regional storage volumes

State	Initial natural surface water storage [GL]	Initial natural groundwater storage [GL]	Initial reservoir storage [GL]
SA	5,321	15,031,350	2,223
VIC	9,040	1,840,000	9,963
NSW	9,040	5,257,000	15,880
QLD	7,030	45,500,000	7,383
ACT	2,061	23,000	147
NT	7,480	8,647	223
WA	368	46,458,150	7,624
TAS	12,207	16,000,000	12,207

source: Australian Bureau of Meteorology [2017], Australian Government [2016c], Lew, Vaillant [2015], Murray-Darling Basin Commission [1999], Department of Natural Resources, Environment, the Arts and Sport [2009]

The initial storages of surface and groundwater are reported in Table 4.3. Surface water storages are divided into natural reservoirs and dams while groundwater storages appear only in their natural form, i.e. in aquifers. It must be noted that the groundwater storages are based on estimations.

4.4.5 Water rights and markets in Australia

Water markets in Australia have gone a long way from their emergence in 1980s, through their expansion in 1990s and early 2000, to the transition to sustainable water markets since 2007. Although Australian water market is increasingly mature, it can still benefit from further reforms to improve efficiency and the availability of information for decision-making of market participants. The largest trading activities occur in the MDB. In particular, interstate trade is possible in the southern connected basin between the various trading zones in NSW, ACT, VIC and SA, as well as between NSW and QLD in the northern parts of the basin. The allowed trading neighbourhoods in this case study are the neighbouring where trading activities exist or where they can potentially exist. The available resources around Brisbane and Sydney are assumed not to be participating in the trading. Instead the states' capitals water demand is met through their desalination plants and existing water treatment plants in proximity. Surface water and groundwater are allowed to be traded.

In this work, the national Australian equivalent terms of "allocation" and "entitlement" are used, where "allocation" is defined as "the specific volume of water allocated to water access entitlements in a given water year or allocated as specified within a water resource plan" and "entitlement" is defined as "exclusive access to a share of water from a specified consumptive pool as defined in the relevant water plan" Australian Bureau of Meteorology [2016d]. Allocation trade involves transferring a volume of water allocation from a seller to a buyer. Allocation trade is allowed when its volume is equal or lower than the amount of unused allocated water of the seller [Victorian Water Register, 2017].

TABLE 4.4: Regulated entitlements per state and rural water supply

State	surface water entitlements [GL]	groundwater entitlements [GL]	rural water consumption [GL]
SA	844	530	161.7
VIC	4,729	870	1,874.0
NSW	9,940	1,154	3,160.3
QLD	4,705	899	1,541.6
ACT	75	1	0
NT	132	126	0
WA	946	1,491	167.6
TAS	1,650	0	33.3

source: Commission [2010], Australian Bureau of Statistics [2015b]

The entitlements reported in Table 4.4 are the rights to withdraw water from surface and groundwater sources. The Tasmanian licences largely consist of unregulated surface water entitlements. Because of the year-round availability of water in Tasmanian rivers, complemented by releases from the hydro-electricity generation scheme, flow volumes largely exceed urban and irrigation demand. As the entitlements are given for both, urban and rural water consumption, the latter is taken into account under the assumption it will change insignificantly within the planning horizon. Hence, there has been no need to issue entitlements that could be limited by allocation announcements. Entitlements are allocated on 1st July every year which is considered the beginning of the water market year. Therefore, the start and end of the time periods are adjusted to match the water market year in Australia. It is worth mentioning that Australia does not import water from abroad. It is assumed that the entitlements remain steady throughout the planning horizon and that carry-overs are possible for all states. It must be noted that there is a maximum volume that can ensure sustainable abstraction. Surface water withdrawals are also constrained by a maximum yield (Table 4.5).

Two major grades of water depending on their reliability exist, i.e. high and low. However, the prices are expressed in volume weighted average price. This is the agreed price among entities exclusive of transaction costs. Prices of allocation trades are determined by the value placed on water by buyers and sellers in response to factors such as purpose of water use, weather patterns, available allocations, jurisdictional arrangements, etc. The trading prices in each state are determined following a number of assumptions: (i)

Table 4.5: Maximum regional sustainable withdrawal limits

State	surface water sustainable abstraction limits [GL]	groundwater sustainable diversion limits [GL]
SA	750.8	1,979.2
VIC	6,326.2	3,355.5
NSW	6,010.0	5,914.4
QLD	3,244.0	2,693.1
ACT	18.0	17.7
NT	54.4	5,476.4
WA	856.8	7,223.5
TAS	3,542.7	2,530.8

source: Harrington and Cook [2014]

the prices have been derived using historical data which have been extrapolated; (ii) the price is mostly affected by the rainfall rather than water demand. Reliable recording of groundwater temporary trading exists, for instance, only in two cases in WA: 51 USD/ML and 165 USD/ML [Legislative Assembly Committee, 2000]. These prices are similar and in the range of surface water trading prices and therefore, taken as values for groundwater allocation trading prices. Inter-state transfers have trading price that includes applicable transaction costs or the so called gross transfer price. The transaction cost, which is charged by the selling state, is based on percentages from the total trade cost, reported by The Allen Consulting Group [2006]. These percentages for each state are NSW - 3.1%, VIC - 2.7%, SA - 21%. Further, it is assumed QLD, NT and WA charge 3.5% from the trade price.

4.4.6 Operating and capital costs

Three options for installation and expansion capacities of each plant type are provided and reported in Table 4.6. The respective capital costs are estimated from correlations obtained from data observations and from economies of scale expressions [Independent Pricing and Regulatory Tribunal, 2011]. For the capital and operating costs it is considered the seawater desalination plants operate with high salinity rejection reverse osmosis membranes while the groundwater treatment plants utilise brackish water reverse osmosis membranes as desalination technologies. A conversion rate of 1 AUD = 0.754 USD is adopted [XE, 2016].

It is assumed it takes two years to build a surface water treatment or groundwater treatment plants, and four years to install a seawater desalination plant. It is also assumed that an expansion of any plant and building a dam take a year. Only installation

Table 4.6: Capacities for plants installation, expansion and respective costs per state

Plants type	Installation		Expansion		Operating costs	
	Capacity [ML/y]	Capital cost [M USD]	Capacity [ML/y]	Capital cost [M USD]	Fixed [USD/ML]	Variable [USD/ML]
SWTP	50,000	52.32	10,000	10.75	528.6	1,233
	100,000	84.67	25,000	24.53	528.6	1,233
	200,000	149.38	50,000	45.78	528.6	1,233
GTP	20,000	191.74	10,000	43.94	585.9	1,367
	50,000	479.35	25,000	100.23	585.9	1,367
	100,000	958.70	50,000	187.04	585.9	1,367
SDP	50,000	970.00	50,000	456.18	2,000	1,386
	100,000	1,943.60	100,000	851.27	2,000	1,386
	150,000	2,916.60	150,000	1,226	2,000	1,386

source: Wittholz et al. [2008], Urban Water Cycle Solutions [2015], Campbell and Brown [2003]

Table 4.7: Capacities for dams installation and respective costs per state

State	Capacity [GL]	Capital cost [M USD]	State	Capacity [GL]	Capital cost [M USD]
SA, ACT	1,000	756	NT	500	378
	2,000	1,512		1,000	756
	3,000	2,268		2,000	1,512
VIC, QLD, WA, TAS	5,000	3,780	NSW	10,000	7,560
	10,000	7,560		20,000	15,120
	15,000	11,340		30,000	22,680

source: [Australian Government, 2014]

of total dams capacity per state is considered. Table 4.7 shows the options of capacities and their respective costs. The operating costs for dams are assumed to be 120 USD/ML [State Government Victoria, 2011].

The capital and operating discount factors are calculated using a discount rate of 6%, which is commonly used in water and wastewater treatment, desalination and water sanitation [Souza et al., 2011, Whittington et al., 2008].

4.5 Computational results and discussion

In this section are discussed the computational results and performance of the single solution approach presented in Section 4.3 and applied to the case study described in Section 4.4. The MILP models are implemented in GAMS 24.7.1, using solver CPLEX 12.6.1, on a PC with Intel Core $i7 - 3770$ CPU 3.40 GHz, RAM 16 GB. The relative optimal gap has been set to 0.01%.

The model is comprised of 78,529 equations, 70,177 continuous and 19,550 discrete variables. The solution is returned within 823 seconds with an objective function of 327.94 bnUSD. A breakdown of the total cost is given in Table 4.8, alongside with total regional costs. Forty two water treatment plants are expanded and one new plant is built

TABLE 4.8: Discounted cost components and regional costs of the optimal water management design

Cost component	[bnUSD]	State	Regional cost [bnUSD]
Capital expenditure of installed/expanded plants and dams	2.33	SA	14.49
Operating expenditure of plants and dams	320.82	VIC	87.18
Penalties for unmet demand	4.79	NSW	80.75
		QLD	51.99
		ACT	2.90
		NT	3.99
		WA	48.37
		TAS	38.27
Total cost	327.94		327.94

in the light of the increasing 25-year period demand, which is reflected in the capital cost expenditure, shown in Table 4.8. The ongoing costs for operating water services account for approximately 95% of the total cost. In OECD [2009], the Australian gross domestic product of total water and wastewater services per year have been reported with average annual expenditures of 6.86 bnUSD by 2015 and projected average annual expenditures of 9.95 bnUSD by 2025. Extrapolating the latter estimate for the period 2016-2040, results in approximately 249 bnUSD without expenditure increase and 311 bnUSD with 3 bnUSD increase every 10 years for the total expenditure. Consequently, the solution returned is in the same order of magnitude as the projected costs and roughly 6% off from the second estimation. The occurring difference can be caused by a number of assumptions. Firstly, the reported values in the report by OECD [2009] are average values for provision and maintenance of adequate water infrastructure. Secondly, the expenditure increase assumed is linear which may not be the case in reality. Additionally, the report does not specify the targeted reliability of future infrastructure while optimisation model returns the highest possible reliability which is *geq* 99%. Finally, not accounting for self-supply in the model does not lower the demand hence, decisions for larger and more capacity expansions and build out are made.

The regional costs are reported in Table 4.8, from where it can be observed the highest costs, 87.18 bnUSD, 80.75 bnUSD and 51.99 bnUSD, incur in VIC, NSW and QLD, respectively. Those areas are densely populated and projections shown in Fig. 4.8

manifest a substantial water demand belongs to them, which can explain the difference in total cost in comparison with the rest of the states. The penalty is triggered in 2016-2017 in VIC, QLD, NSW, NT and WA due to the capacity shortage to produce clean water.

In the same year the groundwater abstractions are on average 4 times higher than the annual abstractions for the rest of the periods and the seawater diversions are almost twice as high as the annual intakes towards 2040-2041 (Fig. 4.12). In the figure, it is observed the groundwater abstraction rises steadily, reaching 77 GL/year, while seawater intake increases exponentially to approximately 131 GL/year towards the end of the planning horizon. Although seawater desalination is available, it is not an economically viable option until demand cannot longer be met by conventional water resources. Surface water procurement remains the major source of water provision, and grows steadily for 25 years, starting at 2,534 GL in the first period and ending at 4,972 GL in the last period. This is under the assumption that the total precipitation will remain the same as precipitation in the last 25 years. Diversifying the water source mix is associated with the yearly gradual operating costs increment from 21.4 to 28.8 bnUSD. Fig. 4.12 demonstrates the long-term necessity of alternative water treatment facilities in place in order to prevent the risk of supply shortages.

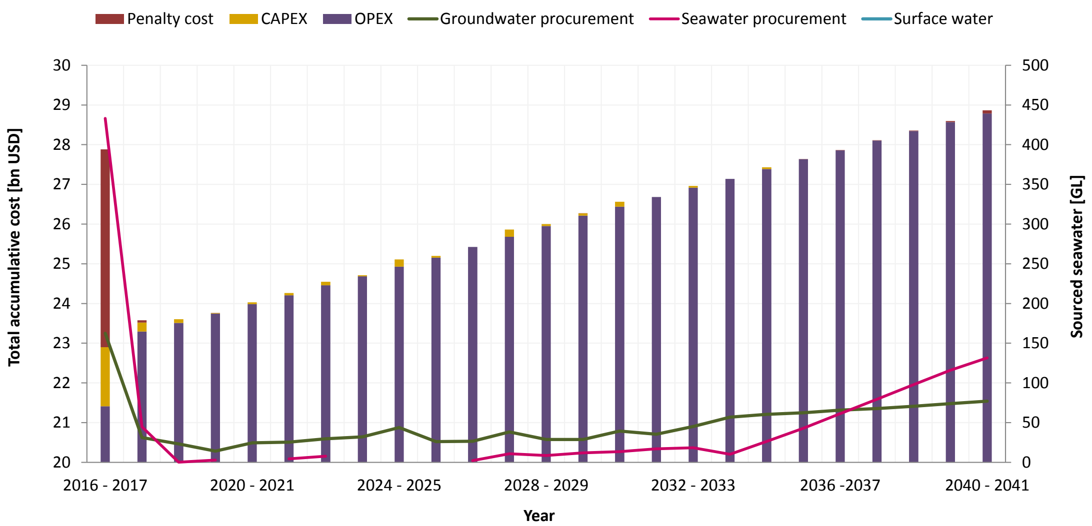


FIGURE 4.12: Components costs and resources intakes in the period 2016 - 2041

Fig. 4.13 illustrates the total regional plant capacity in the period 2016-2041. Water scarcity develops in the areas where the rainfalls are relative to the population. VIC and

NSW, for instance, exhibit lowest average precipitation per capita of respectively 15.3 ML and 45 ML per person. According to Fig. 4.13, both states secure the largest water processing capabilities in Australia in order to mitigate the danger of supply failures. The highest step-changes are made by QLD from approximately 717 GL/y to almost 1,342 GL/y, by VIC from 1,043 GL/y to 2,343 GL/y, and by WA from 508 GL/y to 1,158 GL/y production capacities. The three states which have the largest total costs also possess the largest production capacities, followed by WA. Although NSW necessitates 375 GL/y of extra capacity for the entire planning horizon, the operation of its already existing facilities contributes to its cost. In 2040-2041, the water demand for QLD, VIC and WA is estimated at, respectively, 960 GL, 1675 GL and 805 GL, including distribution losses. The plants' utilisation in the three states is kept at or above 70% at the last year of the planning span. ACT and NT necessitate two expansions each, of 20 GL/y total additional capacity in the former state, and 35 GL/y in the latter. SA possess enough plant capacity to be able to meet its increasing demand therefore, no installations or expansions are needed in the state. Its plants operate at 45% of their capacities in 2016-2017, and at 54% of their capacities in 2040-2041. It must be noted that maximum two expansions per plant have been allowed, which are preferred over installations of new plants due to their lower cost and shorter building period. The options for capacities have been provided taking into account real capacities of each plant type, translating into the smaller and more frequent selection of capacities expansions, as seen in Fig. 4.13.

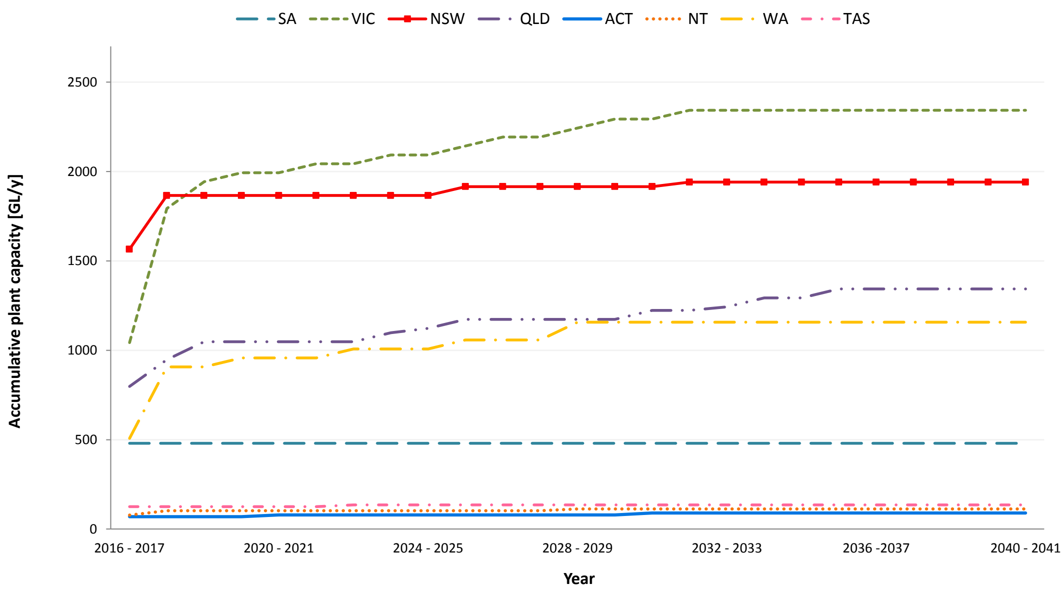


FIGURE 4.13: Total regional plant capacity expansions in the period 2016 - 2041

Fig. 4.14 illustrates the regional water source mix in year 2040-2041. The size of the bubbles is relative to the total plants capacity in a state, meaning the bubbles, which are larger than the one in the legend, have a production capacity larger than 550 GL/year and vice versa. The results show a portfolio of procured resource types where surface water plays a predominant role. Approximately 4% of the urban water demand in VIC and 2% in QLD is met through desalinated water. WA counts approximately 1% on seawater desalination while NT relies on 5% of groundwater. TAS and SA have solely surface water in their water mix to provide urban water supply. Fig. 4.14 resembles the regional water source mix presented in Fig. 4.7 for year 2014-2015, which shows an agreement with current practices as historical hydrological and availability data have been used with a final year 2015-2016. The reason for the slightly stronger preference towards surface water treatment can be explained not only with the cheapest purification cost but also with the extensive trading among the states.

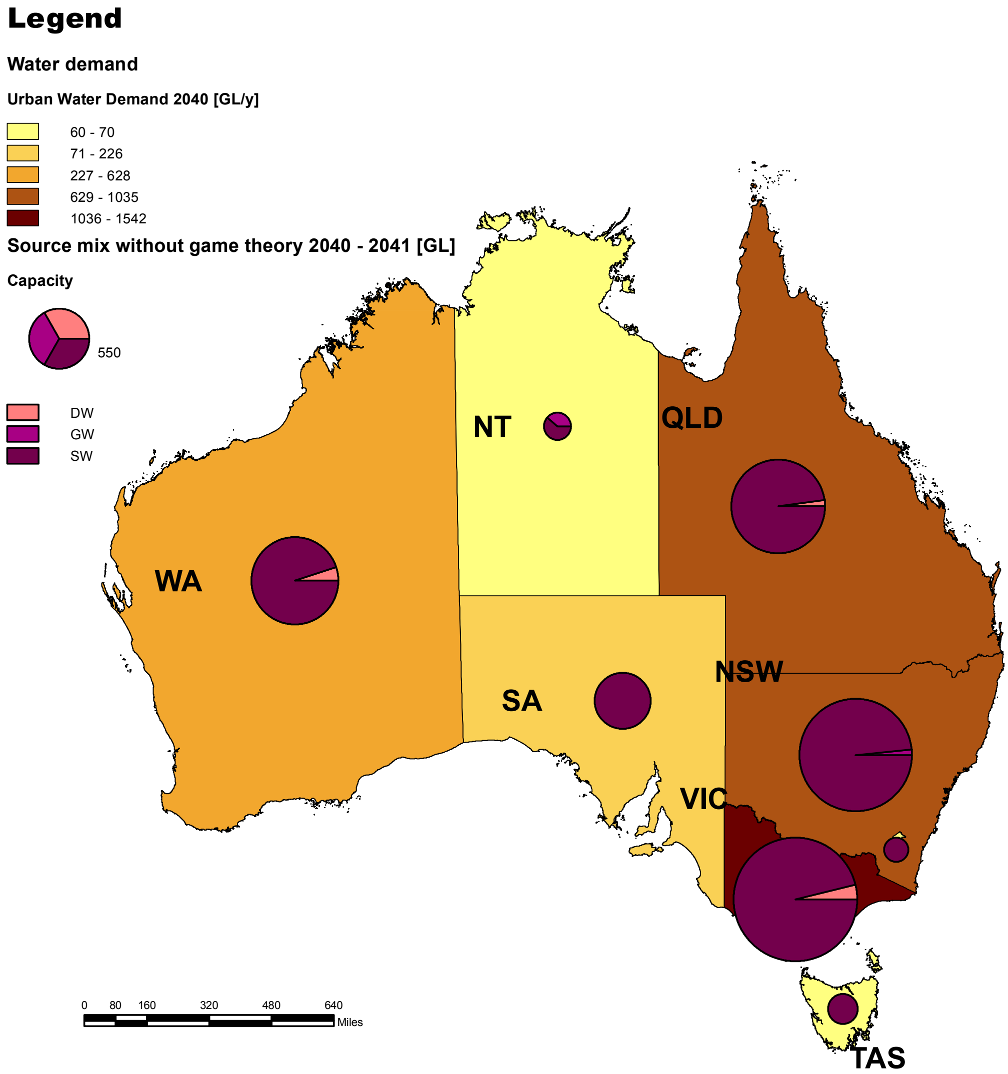
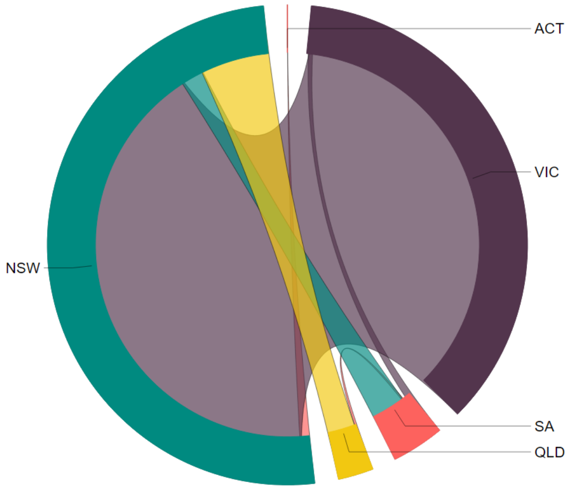
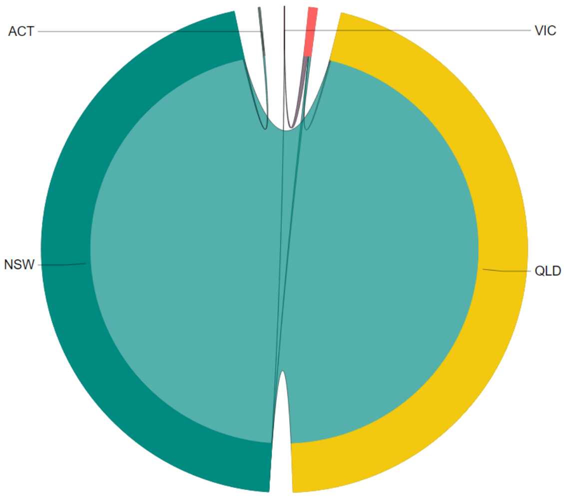


FIGURE 4.14: Water resource mix in 2040 - 2041

It has been allowed SA, VIC, NSW and QLD to be able to trade with its neighbouring states where there is a hydrological connection in MDB. Additionally, Sydney and Brisbane are isolated from trading and they are assumed to provide services only through their locally existing plants and through building new infrastructure. Surface water and groundwater, which are the current transferable sources in Australia, are allowed to be traded. The total surface water and groundwater volumes traded in and out from each state are depicted in Fig. 4.15(a) and Fig. 4.15(b), respectively, and summarised in Table 4.9. The darker colour shades at the rim of the circles represent each state and the respective lighter coloured chords correspond to the flows that are sold by that state. The arc length is indicative of the amount of water sent out from that region. Hence, it can be deduced that the highest trading surface water activities take place between NSW (72,047 GL sold in total), VIC (51,449 GL sold in total) and SA (5,100 GL sold in total). On average, surface water trading provides from 8% up to 30% of the water demand in the country. In Fig. 4.15(b) the volumes as a whole are significantly lower which is due to the environmental restrictions for groundwater abstractions and to the greater costs associated with its treatment. The highest trading activities occur between NSW and QLD with a total sold groundwater of 29,898 GL and 29,903 GL, respectively.



(a) Surface water trades



(b) Groundwater trades

FIGURE 4.15: Total traded volumes of water from state to state

The total regional costs arising from trading per year are shown in Fig. 4.16. In the figure, the positive values count towards a state's expenditures, while the negative values are the money received for selling water and they occur as profit. The low trading at the beginning of the planning horizon is due to the procurement of a region's own sources,

Table 4.9: Regional total traded surface water and groundwater volumes for the 25-year planning horizon

From/	Surface water trades					Groundwater trades				
To	SA	VIC	NSW	QLD	ACT	SA	VIC	NSW	QLD	ACT
SA		861	4,001	236			228	139	8	
VIC	502		50,947			0.1		5		
NSW	2,710	60,010		8,161	1,166		5		29,815	78
QLD	269		3,153			71		29,832		
ACT							85			

such as groundwater and seawater. Surface water is in a higher demand in a dry year, therefore, more transfers happen in those periods, which, on the other hand are coupled with higher transfer prices. From Fig. 4.9 and Fig. 4.11 it can be deduced that periods 2018-2019, 2026-2029 and 2030-2034 are exposed to lower rainfalls and streamflows. In those periods, VIC has trading expenses varying up to to 0.28 bnUSD. On the contrary, NSW and QLD gain profit at various points throughout the planning horizon.

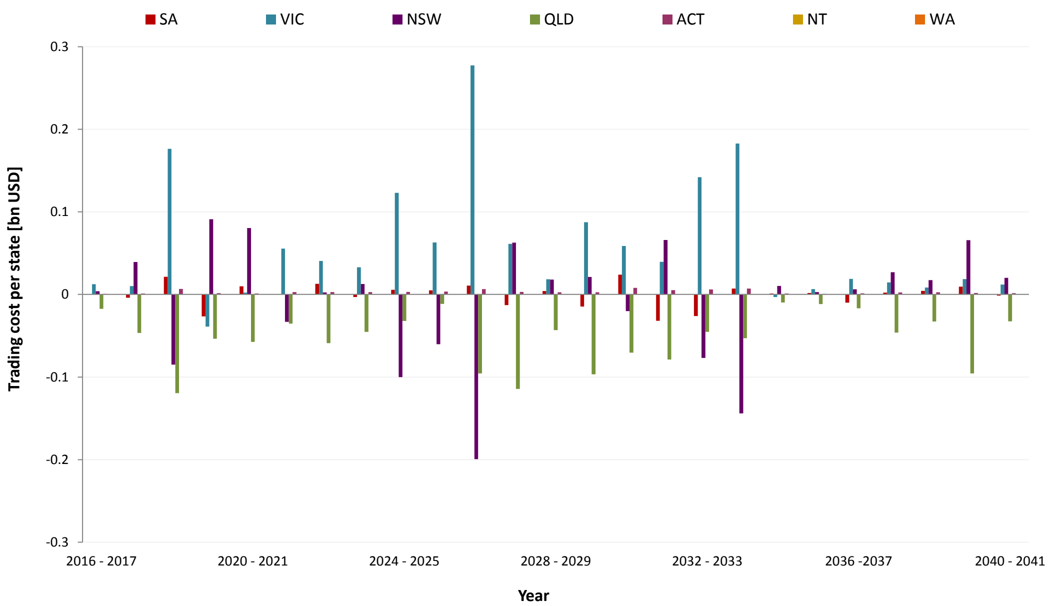


Figure 4.16: Regional trading transactions in the period 2016 - 2041

For a total cost of 327.94 bnUSD, the volumetric supply reliability for the country is 99.44%. So far, Perth have investigated the water supply planning process and incurring costs at a targeted reliability of 90% [PMSEIC Working Group, 2007], which is lower than the obtained value from the model. In years when rainfall is below average in conjunction with water production capacity shortage and increasing demand, reliability that high is uncommon. Further, it has been a historical practice for the industry to agree at an 'accepted level' of reliability with the urban communities, which involves temporal or volumetric restrictions households are subject to. Such an accepted level is set by the communities' willingness to pay for extra security of supply, which is difficult to determine [Hughes et al., 2009]. In order to explore a better and fairer trade-off between the two, the multi-objective optimisation solutions with ϵ-constraint method and game theory are discussed in the next chapter (Chapter 5).

4.6 Concluding remarks

A spatially-explicit multi-period Mixed Integer Linear Programming (MILP) model has been developed for the design and management of water supply system. The optimisation framework encompasses decisions such as installation of new purification plants, capacity expansion, and raw water trading schemes. The objective is to minimise the total cost incurring from capital and operating expenditures in order to meet demand. Assessment of available resources for withdrawal is performed based on hydrological balances, governmental rules and sustainable limits. The applicability of the model has been investigated through a case study based on Australia.

Key findings suggest a trend in plants expansions and trading can keep surface water as the major source in the next 25 years. Nevertheless, diversifying the water source mix benefits from lowering the dependency on precipitation and securely meeting the urban water demand. The possibility of all the neighbouring states situated on Murray-Darling Basin to trade, offers the advantage of providing surface water and groundwater in periods of drought. Supply reliability increases towards the end of the planning horizon, when larger capacities for conventional sources are in place. The results indicate a preference towards expansions to building plants where the majority new infrastructure is located in VIC, QLD and WA.

Chapter 5

Multi-objective Optimisation of Water Management Systems with Supply Reliability

In the light of the increasing importance of reliability, the objective is no longer to only minimise cost, as presented in Chapter 4, but also ensure the system is reliable to an economically adequate level while shortfalls are brought to minimum. This chapter aims to develop multi-objective formulations for obtaining the Pareto-optimal and the fairest solution of all using two approaches.

5.1 Theoretical background

Damelin et al. [1972] first introduced the concept of reliability of water supply in a simulation context. Barlow [1984] presented a historical angle of mathematical theory of reliability. Glueckstern [1999] assessed the reliability of small to medium desalination plants. Koss and Khawaja [2001] conducted a contingent valuation method study on water supply reliability in California and the willingness of customers to pay to avoid shortages. Papadakis et al. [2007] focused on a case study about Northern Greece to demonstrate that adequate water supply planning was needed in order to ensure high supply reliability. Wang and Au [2009] presented Monte Carlo simulations for the probabilistic performance of water supply where reliability varied spatially. Abunada et al. [2014] incorporated demand balancing tanks in network optimisation and reliability assessment into a newly developed Networks Optimisation and Reliability Assessment Tool (NORAT). Gupta et al. [2014] assessed reliability of supply based on shortfall of water distribution networks using node flow analysis. Peng et al. [2015] presented a mathematical formulation for water allocations accounting for reliability. Reliability has also been the focus of numerous works which consider it alongside calamities and changing climate [Wang and Au, 2009, Simonit et al., 2015, Clark et al., 2015, Yoo et al., 2016].

Multi-objective optimisation approaches have been the focus of a large number of literature works. Pokharel [2008] was one of the first works to use multi-objective optimisation in supply network design where two-objective decision-making model for the choice of suppliers and warehouses for a supply chain network design was proposed. Amodeo et al. [2009] integrated evolutionary algorithms and supply system simulation for the maximisation of customer service level and the total inventory cost. Liu and Papageorgiou [2013] developed an MILP model for cost, responsiveness and customer service level using ϵ-constraint method and lexicographic minimax method as solution approaches. Chen and Andresen [2014] applied a weighted-sum approach minimising costs, emissions, and employee injuries in a supply system. Fraga et al. [2017] presented a dynamic programming model for the infrastructure decisions versus reliability. Campana et al. [2017] proposed a multi-objective genetic algorithm for an energy-water framework to minimise the system life cycle costs, and maximize renewables and water harvesting reliability.

When a fair strategic decision is sought in a multi-objective problem, game theory is most commonly applied. Game theory can be utilised for various applications, such as engineering, life sciences, management and economics. Games can be collaborative, when the best strategies for the players are to cooperate, and competitive, when the players can maximise their outcome if they do not take into consideration the outcomes of the rest of the players. Games can also be simultaneous and sequential, when the decisions of the players are taken at the same time or one after another, like in a leader - follower type of game. The former often implies the information is not well known and in cases of the latter, normally the follower makes a decision based on the action of the leader. This leads to dealing with perfect and imperfect information games. Recent works on game theory in mixed integer programming have been classified qualitatively based on the aforementioned applications. A typical leader - follower game is the Stackelberg game which has been the chosen strategy in different literature sources [Yue and You, 2014, Bard et al., 2000, Yang et al., 2015, Pita et al., 2010, Yin, 2013]. Zhang et al. [2013] developed mathematical models for fair electricity pricing microgrid, scheduling, planning, and in Zhang et al. [2017] - carbon capture and storage following cooperative Nash approach [Nash, 1950].

Definition

"Nash approach rests on the situation of bargaining where individuals or strategies have the opportunity to collaborate for mutual benefit in such a manner that no action taken by one agent can affect the well-being of the other one. "

Nash equilibrium has been applied in supply chains and scheduling [Zamarripa et al., 2013, Gjerdrum et al., 2002, Banaszewski et al., 2013, Pira and Artigues, 2016, Ortiz-Gutierrez et al., 2015, Tushar et al., 2014]. Supply chain game theory and transfer prices have been covered by Simchi-Levi et al. [2004], Rosenthal [2008]. Additionally, Shelton [1997], Tambe [2012] have published exhaustive compilation books on game theory, security and markets. Madani [2010] compiled a literature review on game theory concepts applied to water resources management. Sechi et al. [2011] suggested a decision making tool using game theory to determine fair water pricing with sustainability principles. M. Daumas and Ventou [2009] proposed a mathematical model for the theory of co-operative games for transferable utilities. [Souza Filho et al., 2008] investigated game theory on water users' strategic behaviour. Nikjoofar and Zarghami [2013] simulated water distribution networks using multi-objective optimisation and game theory.

In this chapter, a multi-objective optimisation is formulated from the mathematical formulation presented in Chapter 4. The objectives are the simultaneous minimisation of total cost and maximisation of reliability using ϵ-constraint method. Nash bargaining approach is then used to determine the fairest operating point from the optimal Pareto front.

5.2 Problem statement

The supply chain problem replicates the description in Chapter 4. In addition, strategic decisions re made for the allocation of water resources, procurement and treatment of sources types, locations and capacities augmentations for dams and treatment plants, trading directions and volumes for setting a specific country's reliability of supply target.

Assumptions

- Volumetric reliability can represent accurately reliability of supply
- Absence of water management plan means no infrastructure and no trading are taking place

Hence, the problem can be stated below.

Given:

- geographical divisions into regions/states/territories
- planning time horizon, e.g. a 25 - year horizon
- water sources, i.e. surface water, groundwater, seawater, etc.
- final water uses, i.e. urban, rural, etc., and seasonal demand over planning horizon
- regional and seasonal climatic data, i.e. precipitation, evaporation, run-off, streamflows
- initial water storages in drainage basins and reservoirs
- geographical distribution, capacities, operating efficiencies, and operating and capital cost parameters of existing and potential dams and plants
- maximum allocated water sources per end-use, i.e. entitlements
- trading topology and prices options
- inflation and discount factors
- regional sustainable diversions/abstractions
- penalty costs for not meeting demand
- a set of minimum supply reliability values

Determine:

- available water sources for diversion/abstraction

- procurement rate for each water source and end-use water production rate
- trading and carry-over flowrates
- location and capacities of new dams and plants installations, and existing plants expansions

So as to: minimise total cost for the design of the water supply chain and maximise the reliability of supply. The problem is formulated as a multi-objective spatially-explicit multi-period MILP model. Two solution approaches are implemented next, i.e. an ϵ-constraint method and a game theoretic approach.

5.3 Mathematical formulation

In this section, reliability of supply is added as a second objective function to the optimisation framework presented in Chapter 4. The problem is solved using an ϵ-constraint method in Section 5.3.1, and game theory in Section 5.3.2. A multi-objective optimisation for minimising total cost and maximising reliability of supply is going to determine the extent the supply chain network design is influenced by both factors. Additionally, game theory will provide a fair trade-off between the two.

5.3.1 ϵ-constraint method

An ϵ - constraint method is applied for the solution of the multi-objective optimisation where the first objective is to minimise the total cost for the supply system and the second objective is to maximise the reliability. Opposed to the weighted sum method, the ϵ - constraint method is suitable as the relative importance of each objective is unclear. Furthermore, the method will result in an evenly distributed Pareto frontier. In the ϵ - constraint approach, the cost objective remains as it is while the remaining objective is turned into inequality with a set of lower bounds. The reliability, however, is implicitly related to the penalty, $OPen_t$, in Eq.(4.38), which is the reason it has to be excluded from the objective function of the total cost. Hence,

$$Objective\,1: \quad minimise \;\; TC = \sum_t (cdf_t \cdot CAPEX_t + odf_t \cdot OPEX_t) \tag{5.1}$$

which is subject to:

$$Objective\,2: \quad WR \geq eps \tag{5.2}$$

and

- hydrological and supply-demand balances Eq.(4.3) - Eq.(4.7)
- procurement constraints Eq.(4.8) - Eq.(4.14)
- reliability constraints Eq.(4.15) - Eq.(4.16)
- capacity constraints Eq.(4.17) - Eq.(4.26)
- production constraints Eq.(4.27) - Eq.(4.30)
- capital expenditure constraints Eq.(4.35) - Eq.(4.37)
- operating expenditure constraints Eqs.(4.31),(4.32), Eq.(4.34)

The obtained solutions will be Pareto optimal and any of them can be chosen to plan the water supply chain. The Nash bargaining approach, however, can provide the exact point on the Pareto curve where the two strategies can co-exist at equilibrium.

5.3.2 Nash bargaining approach

A cooperative game is considered to obtain the best strategies for expenditures and supply reliability using Nash bargaining approach. The deployment of the method is necessary as to investigate whether and how a satisfactory agreement between the two strategies could be reached. It is aimed to minimise total country's cost by increasing the difference between the status quo point and the optimisation variable. On the other hand, it is aimed to maximise the reliability by increasing the difference between the variable and its status quo point. The status quo point represents the situation where both agents will not be able to achieve an agreement. By maximising the product of all the strategies' deviations, a fair solution distribution is ensured where no strategy can be improved. Two relevant axioms stem from classical theory: (i) none of the strategies will deteriorate from the status quo pay-off, or individual rationality axiom and (ii) the solution could not be improved on to both strategies' advantage, hence, Pareto optimal solution is obtained. The dependency is expressed in Eq.(5.3).

$$maximise \qquad \bar{\tau} = (WR - WR^{quo}) \cdot (TC^{quo} - TC) \tag{5.3}$$

where TC^{quo} is the upper cost bound for the country, which is obtained in a case no infrastructure is planned and no trading occurs. Then, $TC \leq TC^{quo}$. WR_{quo} is the second point for the status quo pair. Then, $WR \geq WR^{quo}$. Eq.(5.3) results in a non-linear formulation which can result in local optima. Therefore, it follows to be further linearised. Eq.(5.3) is expressed as a separable function by taking the logarithm of both hand sides and using logarithmic properties:

$$ln\bar{\tau} = ln(WR - WR^{quo}) + ln(TC^{quo} - TC) \tag{5.4}$$

Then, an additional parameter, ξ_k is introduced to equal the logarithm of the cost difference (Eq. (5.5)).

$$\xi_k = ln(TC^{quo} - TC_k), \forall k \tag{5.5}$$

where TC_k is a parameter representing option k for the total cost. A parameter, λ_k is assigned for the logarithm reliability difference, shown in Eq.(5.6).

$$\lambda_k = ln(WR_k - WR^{quo}), \forall k \tag{5.6}$$

where WR_k is a parameter representing option k for the normalised reliability. An SOS type 2 variable, X_k, is used to represent the selection of the cost, shown below:

$$\sum TC_k \cdot X_k = \sum_t (cdf_t \cdot CAPEX_t + odf_t \cdot OPEX_t) \tag{5.7}$$

The same variable is used for the reliability, expressed below:

$$\sum WR_k \cdot X_k = \sum_{i \in W} \sum_g \sum_t \sum_q WSR_{igtq} / (G^{max} \cdot T^{max} \cdot Q^{max}) \tag{5.8}$$

The active option k should add up to 1, represented in Eq.(5.9).

$$\sum X_k = 1 \tag{5.9}$$

And the auxiliary variable has to be positive.

$$X_k \geq 0, \forall k \tag{5.10}$$

Then, the objective function becomes:

$$maximize \qquad \hat{\tau} = \sum_{k=1}[(\xi_k + \lambda_k) \cdot X_k] \tag{5.11}$$

which is subject to:

- hydrological and supply-demand balances Eq.(4.3) - Eq.(4.7)
- procurement constraints Eq.(4.8) - Eq.(4.14)
- reliability constraints Eq.(4.15)
- capacity constraints Eq.(4.17) - Eq.(4.26)
- production constraints Eq.(4.27) - Eq.(4.30)
- capital expenditure constraints Eq.(4.35) - Eq.(4.37)
- operating expenditure constraints Eqs.(4.31),(4.32), Eq.(4.34)
- game theory constraints Eq.(5.7) - Eq.(5.11)

The applicability of the mathematical models is investigated through an illustrative example.

5.4 Illustrative example

The case study of Chapter 4 is adopted for consistency purposes.

5.5 Computational results and discussion

In this section are discussed the computational results and performance of the multi-objective solution approaches presented in Section 5.3 and applied to the case study described in Section 4.4. The MILP models are implemented in GAMS 24.7.1, using solver CPLEX 12.6.1, on a PC with Intel Core $i7-3770$ CPU 3.40 GHz, RAM 16 GB. The relative optimal gap has been set to 0.1%.

5.5.1 ϵ - constraint multi-objective optimisation

For the ϵ - constraint method, 11 MILP problems are solved with an average CPU time of 11 seconds and a total CPU time of 120 seconds. At WR = 0, the total cost contains the fixed operating cost of the existing plants, 159.6 bnUSD. Until 174.5 bnUSD, the total cost increases gradually while no capital expenditures from newly built plants contribute to it. That point corresponds to a supply reliability of 40%. From that point onwards, the cost grows almost exponentially until it reaches 323.3 bnUSD with a maximum reliability achieved - 99.5%. The obtained Pareto curve is plotted in Fig. 5.1, demonstrating all the optimal solutions, possible for the supply chain design and operation. The decision of the local governments and authorities to determine the point where they would like to stand is an intricate task. Hence, applying game theory can find the exact point where cost and reliability are at equilibrium.

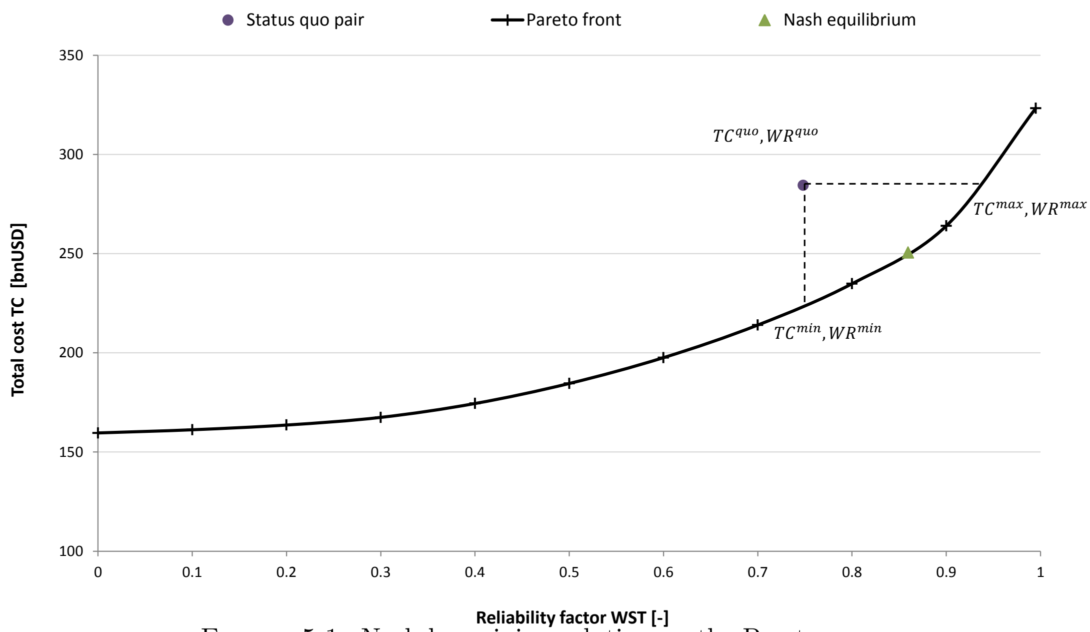


FIGURE 5.1: Nash bargaining solution on the Pareto curve

5.5.2 Nash bargaining approach

The choice of a status quo pair(s) (WR^{quo}, TC^{quo}) in the Nash bargaining approach would define the outcome of the game theory. To select the two pay-offs, it is assumed no agreement can be settled between the two strategies, total cost and supply reliability. Hence, a worst case scenario is adopted where no improvement of reliability through building new infrastructure and water transfers can be achieved. Simultaneously, it is desired to maximise the reliability subject to the cost. WR^{quo} is equivalent to WR^{min} while TC^{quo} is equivalent to TC^{max} (Fig. 5.1). In order to find out the negotiation set, where $WR^{quo} \leq WR \leq WR^{max}$ and $TC^{min} \leq TC \leq TC^{quo}$, and the pair (WR, TC) is Pareto optimal, WR^{max} and TC^{min} are obtained. WR^{max} is the value obtained when reliability is maximised at $TC = TC^{max}$ whereas TC^{min} is found by minimising the total cost subject to $WR = WR^{min}$. The separable approach is executed using 100 discretisation points taken from WR^{quo} to WR^{max} and the corresponding points from TC^{min} to TC^{quo}. The maximum bargaining solution is shown in Fig 5.1 and reported in Table 5.1.

Table 5.1: Nash bargaining approach solutions

	Objective values		CPU [s]
	Water supply reliability WR [-]	Total cost TC [bnUSD]	
Status quo pair	0.748	284.43	5
Max WR/ Min TC	0.944	223.41	100/ 20
Nash approach	0.859	250.45	396

From Fig. 5.1, it can be observed that the solution lies in the middle of the subset of optimal solutions considered. Reliability of 85.9% translates into a total cost of 250.45 bnUSD. The pay-off where the two strategies are in equilibrium coincides with a point on the Pareto front. The Nash bargaining solution is optimal because it is obtained from the maximum product of two strategy gains and following from the second classic axiom presented earlier, this product will attain a Pareto-optimal solution. The value for reliability has worsened by 14% and total cost value has improved by 25% from the monolithic approach. It must be noted that if a different methodology for deriving the status quo pair is used, the results obtained will differ.

The corresponding capacity expansions for the Nash equilibrium are illustrated in Fig. 5.2. From the figure, it can be deduced the expansions spread out throughout the planning horizon instead of taking place at its beginning, as seen in Fig. 4.13. The delay in the decisions is due to the compromise in supply reliability where decisions for augmenting the infrastructure are made at the times when the reliability would otherwise deteriorate. At the end of the planning horizon VIC reaches a final total capacity of approximately 1,100 GL/y, 1,200 GL/y less in comparison with the monolithic approach. QLD and WA reach production capacities of 1,342 GL/y and 1,108 GL/y, respectively.

As the supply reliability is normalised for the entire country, it is observed VIC undergoes largest cuts in reliability due to needed production capabilities.

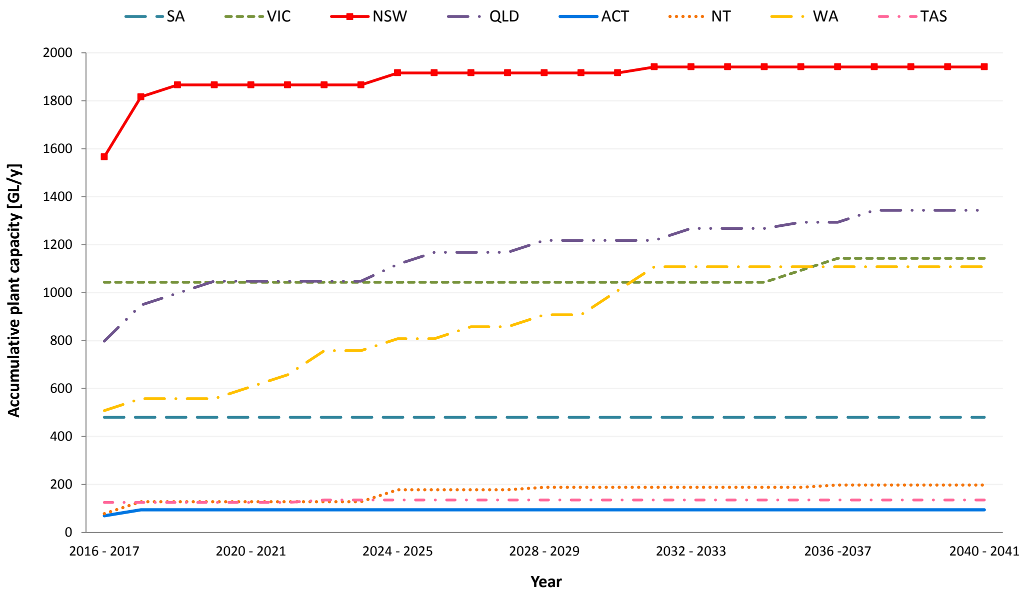
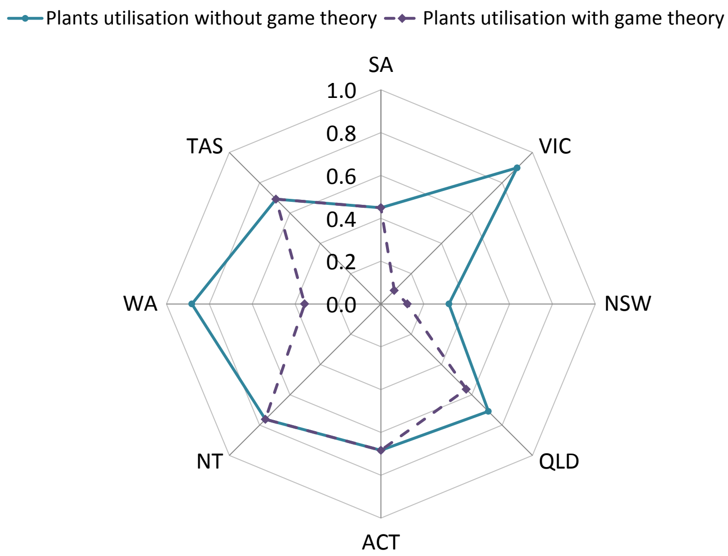


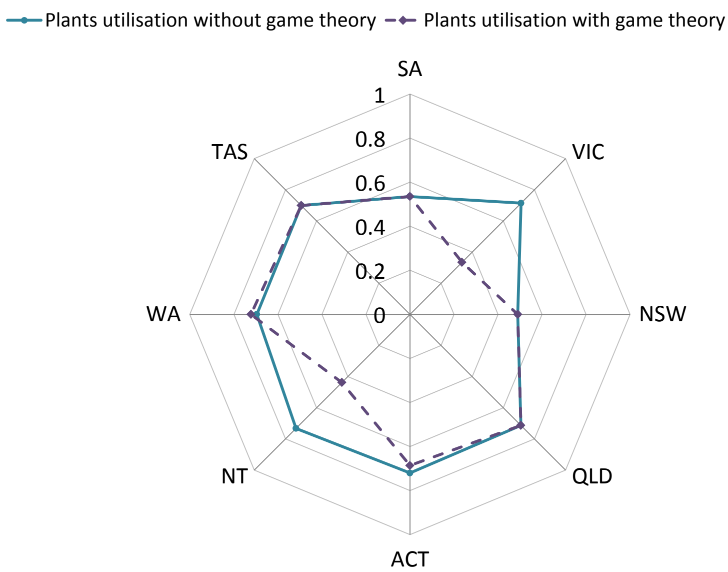
FIGURE 5.2: Total regional plant capacity expansions in the period 2016 - 2041 under game theory

The plants utilisations for the first and last year, for both, the monolithic approach and game theory, are shown in Fig. 5.3(a) and Fig. 5.3(b). From Fig. 5.3(a), it can be observed the difference of the plants utilisation in the monolithic approach and game theory throughout the first year of the planning horizon. The states which do not need to expand their capacities coincide roughly with their utilisation for both approaches which appears as a darker area in the figure. VIC and QLD build more capacities in the monolithic model opposed to importing water while in Nash bargaining approach not all of the available capacity in NSW is utilised in order for variable operating costs to be reduced. In 2040-2041, the radar shades coincide better for the two approaches. As demand increases and capacities have to be built, both models add capacities. It has already been seen, however, that for the game theoretic approach majority of the expansions happen in 2024-2030. Towards the end of the planning horizon, the reliability increases and hence, the utilisation profile of plants. Any shrinkages in the patterns are due to the augmented capacities of plants, which are operating at a higher production rate without reaching their full capacities. As manifested from Fig. 5.3(a) and Fig. 5.3(b), this is the case in VIC, for instance, where at the end of the planning horizon, the utilisation of plants has dropped from almost full operating capacity in 2016-2017 to

71% utilisation of plants in 2040-2041 for the monolithic approach, and the utilisation has increased from 9% to 34% for the game theoretic approach.



(a) Plants utilisation in 2016-2017



(b) Plants utilisation in 2040-2041

FIGURE 5.3: Plants utilisation for the first and last year of the planning horizon without and with game theory

5.6 Concluding remarks

The reliability of water supply in the monolithic mathematical formulation in Chapter 4 has become the second objective function in a multi-objective formulation using ϵ-constraint method. The trade-off between total cost and reliability has been determined by using the Nash bargaining approach. The applicability of the model has been investigated through the case study based on Australia (Chapter 4). The results manifest a decrease in total cost from 327 bnUSD to 250 bnUSD, which corresponds to a 14% total supply reliability decrease. These optimal results from game theory indicate the sacrifices in total cost and supply reliability to obtain the fair design between the two objectives. The decisions for capacity expansions are spread out throughout the planning horizon unlike what is observed in the monolithic approach where the decisions are concentrated in the first part of the planning horizon. This gives a set of outcomes for governments to consider in decision making when investing in infrastructure.

Chapter 6

Conclusions and Directions for Future Work

This thesis addresses the design and optimisation of water management systems on two levels, i.e. process design, addressed in Chapters 2 and 3, and supply chains, addressed in Chapters 4 and 5. The former aims to construct a wide spectre-superstructure consisting of the most commonly used treatment technologies in industry. It involves decisions on the topology, technology choice and operating conditions driven by economic performance. The latter integrates supply chains with hydrological, regulatory and reliability aspects to investigate the least cost intensive infrastructure in a given country. This chapter aims to draw the major conclusions of the work presented in this thesis and provide potential directions for future work.

6.1 Concluding remarks

In Chapter 2 a systematic approach for the design of water and water-related treatment processes using superstructure optimisation has been proposed. The optimisation framework has been formulated as an MINLP model where the major non-linearities arise from removal efficiency, mass balances, and cost constraints. The objective has been the minimisation of total production cost while simultaneously maximising the production flow. Two case studies with applications on seawater desalination and advanced wastewater treatment have been discussed. Sensitivity analysis has shown flowsheets are most sensitive for various TSS concentrations. Preference over membrane technologies for pre-treatment is seen which is a global trend today. The computational results have demonstrated an agreement with industrial flowsheets and production costs.

Chapter 3 has added alternative paths to the superstructure in Chapter 2, which has resulted in a highly non-linear MINLP model. To overcome the model instability, key bilinear terms and non-linear functions have then been reformulated, and the plMINLP model has been introduced. Finally, the MILFP model has been proposed, which includes further discretisations of continuous domains together with a two-step iterative solution procedure based on Dinkelbach's algorithm. The three methods have been tested and compared in an illustrative example of seawater desalination and surface water treatment. The proposed MILFP model has taken the upper hand with respect to CPU times and solution quality despite the 30 times increase of model size. In comparison with the formulation in Chapter 2, the objective function decreases due to the flexibility of recovering a portion of the concentrate, which is also a preferable option, in particular, in industries counting on membrane filtration.

In Chapter 4 a spatially-explicit multi-period MILP model has been developed for the design and management of water supply chains. The features in the proposed optimisation framework cover hydrological balances which can be used for the determination of water storage and seasonal availability of water. On the other hand, temporal allocations and trading schemes are also governed by the availability of water in a given area. Decisions entail the volumes and time periods for production capacity augmentations in order to meet urban water demand at minimum total country cost. The applicability of the approach is investigated in a case study based on Australia. Expansions and installations of predominantly surface water treatment plants with more significant overtake of seawater desalination towards the end of the planning horizon is observed. As opposed to the general view of a growing need of desalination in Australia, the model selects the most economically suitable build options. However, it has to be kept in mind, the hydrological data taken is historical which shifts the technologies' choice.

In Chapter 5 a second objective has been included to the objective function in Chapter 4 to account for the reliability of water supply. Two methods have been applied as solution methods, i.e. ϵ-constraint method and Nash bargaining approach. The former has been used for deriving the Pareto-optimal front. A status-quo situation is assumed when no negotiation can exist between reliability and cost, and Nash equilibrium finding the fairest trade-off between the two has been located on the Pareto curve. The solution has moved to a 24% lower cost and 14% lower reliability values in comparison to the solution in Chapter 4.

6.2 Directions for future work

This thesis has examined topics of process design and supply chains, and although it has attempted to cover various aspects from both, the work is subject to limitations. Furthermore, it can be extended in several research directions as future work as follows:

Chapter 2 and Chapter 3

- The presented superstructures can be extended to accommodate primary and secondary wastewater treatment, as well as sludge treatment. Hence, an integrated process design and partially self-energy supplying system would be able to be investigated.
- It has been determined that variation of input results in different flowsheet configurations. Design with input uncertainty could be a future possible direction of this work which is particularly important in diurnal and seasonal variations in concentration.
- Membranes are the preferred technology taking place in water treatment design. Their environmental burden, however, should not be ignored. Life cycle assessment of the employment of the membranes can contribute to a more precise cost estimation. Thus, a shift in technologies is likely to be observed.
- Removal efficiencies have been modelled through regressions. Surrogate models if substituted with first principle models will allow for more accurate removal representation.
- Metaheuristic methodology can be implemented as a black box function to simulation procedures to obtain output performance measures of the model.

- Addressing all of the above will inevitably increase the computational burden of the model. Benders decomposition approach as a solution procedure is applicable due to the distinctive blocks of technologies involved in the superstructure.

Chapter 4

- The problem statement involves common sources, purification methods and urban water as an end use. A future area of improvement may consider the extension of the superstructure to capture more water sources, such as reclaimed water, treatment plants installation options such as wastewater treatment plants, and end users, such as industrial and rural usages.
- Transportation costs, which account for a significant proportion of water management cost, were not part of this work. Taking into consideration piping and pumping will also influence the decisions regarding water infrastructure. They will be useful to be included in the future as to obtain a more comprehensive economic picture.
- Demand and hydrological inputs uncertainty through stochastic optimisation would contribute to the framework by designing a more flexible infrastructure. Furthermore, predictions rather than historical hydrological data will alter the choice of building technologies.
- Engineering psychology and the human preferences aspect of determining prices, treatment options, etc. will be an interesting domain in the supply chains design.

Chapter 5

- Volumetric reliability is in the focus of this work. Volumetric versus temporal reliability, however, can be examined next as future work.
- The method of determining the status quo in this work is not the only one possible. Different methods for determining the status quo pair can be looked at, for scenarios with and without trading, and with and without infrastructure decisions, for instance, in order to determine which is the least fair of all, i.e. that will provide a better starting point for Nash equilibrium.

- The objective function has been reformulated using a separable approach. Alternative techniques for linearising the objective function can be applied in search for better formulation performance. For instance, the multi-parametric disaggregation technique can be compared against the separable approach to analyse their computational performance.

A number of publications have arisen from the work in this thesis. They are listed next.

Publications

The publications which have arisen from this work are listed below.

Peer reviewed journal publications:

1. Koleva, M.N., Polykarpou, E.M., Liu, S., Styan, C.A., Papageorgiou, L.G., 2016. Optimal synthesis of water treatment processes. Desalination and Water Treatment, 1 – 22

2. Mariya N. Koleva, Craig A. Styan, Lazaros G. Papageorgiou, Optimisation approaches for the synthesis of water treatment plants, Computers & Chemical Engineering, Available online 3 January 2017

3. Koleva, M.N., Calderon, A.J., Zhang, D., Styan, C.A., Papageorgiou, L.G., 2018. Integration of Environmental Aspects in Modelling and Optimisation of Water Supply Chains. Manuscript accepted for publication.

Peer reviewed conference publications:

1. Koleva, M. N., Polykarpou, E. M., Papageorgiou, L. G. (2013). An MILP Model for Cost – Effective Water Treatment Synthesis. Piantadosi, J., Anderssen, R.S. and Boland, J. (eds). Adapting to change: the multiple roles of modelling, 1-6 December 2013, Adelaide, Australia MODSIM, 2716 – 2722

2. Koleva, M. N., Polykarpou, E. M., Liu, S., Styan, C. A., Papageorgiou, L. G. (2015). Synthesis of Water Treatment Processes using Mixed Integer Programming. In: Krist, V. Gernaey, J.K.H., Gani, R. (eds.), 12th International Symposium on Process Systems Engineering and 25th European Symposium on Computer Aided Process Engineering. Elsevier. Vol. 37 of Computer Aided Chemical Engineering, 1379 – 1384

3. Koleva, M. N., Liu, S., Styan, C. A., Papageorgiou, L. G. (2016). Multi-objective optimisation approach for the synthesis of water treatment plants. In: Kravanja, Z., Bogataj, M. (eds.), 26th European Symposium on Computer Aided Process Engineering. Elsevier. Vol. 38 of Computer Aided Chemical Engineering, 2379 – 2384

Conference presentations (abstracts only):

1. Koleva, M. N., Polykarpou, E. M., Styan, C. A., Papageorgiou, L. G. (2014). Overall Process Synthesis of Seawater Desalination. Paper presented to 2014 AIChE Annual Meeting, Atlanta, GA, 16 – 21 November 2014.

2. Koleva, M.N., Liu, S., Styan, C.A., Papageorgiou , L.G., 2016. Design of Water Treatment Processes using Mixed Integer Programming. Paper presented at ChemEngDay UK, Bath ,UK, 30th Mar – 1st Apr, 2016.

3. Koleva, M.N., Liu, S., Styan, C.A., Papageorgiou , L.G., 2016. Optimisation Approach for the Synthesis of Sustainable Seawater Desalination Flowsheets. Paper presented at PSE@ResearchDayUK, London ,UK, 12th July, 2016.

4. Koleva, M. N., Calderon, A.J., Styan, C. A., Papageorgiou, L. G. (2016). Managing the Water 'S' – Scarcity towards Security, Water SDGs and Future Water Management, London, UK, Nov, 2016.

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